TOPSPIN INSTRUCTIONS

- 1. How to start TOPSPIN?
- 2. The TOPSPIN window
- 3. How to open an old dataset?
- 4. How to create a new dataset?
- 5. How to lock and shim?
- 6. How to acquire FID signal and modify acquisition parameters?
- 7. How to process 1D spectrum and modify process parameters?
- 8. How to process a 2D NMR spectrum?
- 9. How to display multiple 1D /2D spectra?
- 10. How to perform multiplet analysis?

1. How to start TOPSPIN

- a. Login using your group ID and password
- b. Double click TOPSPIN icon start TOPSPIN software

2. This is the TOPSPIN window:



3. How to open an old dataset:



4. How to create a new dataset:

a. Click File \rightarrow New; OR click the \square button in the upper toolbar; OR type edc in the command line

In the popup dialog box:

New	×
Prepare for a new initializing its NMR	experiment by creating a new data set and parameters according to the selected experiment type.
NAME	exam1d_13C
EXPNO	1
PROCNO	1
DIR	C:\Bruker\TOPSPIN
USER	guest
Solvent	СДСІЗ 🗸
Experiment	Use current params. 🗸 🗸
TITLE	
13C{1H} AV 3	00 Automation Cholesterylacetate
	OK Cancel More Info Help

- b. Specify name, expno, procno, dir and user
- c. Click the down-arrow of the **Solvent** box to choose a solvent from the list
- d. In Experiment box, select Use current params
- e. Type the dataset title in the **TITLE** box
- f. Type rpar in the command line to choose a parameter set from the list For example: Parameter set name: proton experiment =1_protonstd

Carbon experiment = 1_protonstd Carbon experiment = 1_carbonstd

5. How to lock and shim?

- a. Type **lockdisp** in the command line OR click the [#] button in the upper tool menu to open the lock display window
- b. Type **lopo** in the command line and select a solvent from the popup list,
- c. On the BSMS keyboard:
 - Press the **FIELD** button, and move the lock signal to the center of the lock display window
 - Press the **PHASE** button, and adjust the lock signal in-phase
 - Press the X (or X+Z0), the Y (or Y+Z0), the Z1 (or onaxis+Z1), OR Z2 (or onaxis+Z2) shim buttons, and optimize these shims iteratively to make lock-ring-down pattern observable
 - Press the LOCK button
 - Press the **SPIN** button (for 2D NMR experiments, spin has to be off), and wait for spin indicator to stop blinking
 - Optimize Z1 and Z2 shim iteratively by turning the whirl and observing the lock signal level moving up as high as we can
 - If necessary, press the LOCK GAIN button to decrease/increase lock gain
 - Then press the **STDBY** button
- d. If shim is messed up, type **rsh currshim** in the command line to read most current shim file in
- e. Autoshim: type topshim. In the popup window, choose 1D shim and turn Z6 off, then click start (only for TOPSPIN 2.0 and newer)

6. How to acquire FID signal and modify acquisition parameters

- a. Type **rga** in the command line, then
- b. Type zg in the command line
- c. Sometimes it is necessary to modify acquisition parameters
 - Modify acquisition parameters
 - Clicking AcquPars tab in the tab bar of the data window
 - **OR** type eda in the command line
 - Modify pulse program parameters
 - Click the ¹ button in the toolbar
 - **OR** type **ased** in the command line

Spectrum Proch	Pars AcquPars Title	PulseProg Peaks Integr	als Sample Struct
6 J. S 😸	🖽 83 🔻 Ma		
Experiment	- Experiment		
width	• Experiment		
Receiver	PULPROG =	zgpg30	E Currei
Nucleus	AQ_mod =	DQD	Acquit
Durations	TD =	65536	Size o
Power	NS =	256	Numb
Program	DS =	4	Numb
Probe	TD0 =	1	Loop
Lists	▼ width		
Wobble	SW Inpml =	238 2980	Spect
Lock	SVVH [Hz] =	17985.611	Spect
Missellapeous	AQ ISI =	1.8219508	Acquit
User	FIDRES [Hz] =	0.274439	Fid re
Routing	FVV [Hz] =	90000.00	Filters
	▼ Receiver		

Other buttons in AcquPars toolbar

Set probehead/solvent dependant parameters [getprosol]



U

Set nuclei and routing [edasp]

Change data dimensionality, which will changes the number of parameter columns and value of the acquisition parameter **PARMODE**

7. How to process 1D spectrum and modify process parameters

- a. Modify process parameters
 - Click **ProcPars** tab in the tab bar of the data window
 - **OR** type **edp** in the command line

Spectrum Print	and Arthrain Law	introduced in and a second and	Sargee Structure Fills	
-> 5 III V	25			
Averalise Protein Datasetine Filtagenter Filtagenter	Paterana Si - Si - Si P (Mrs) - OFFEET (pass) - Sin (re) -	22760 75.4677490 219.161 0.00	Table of real spectrum type://committer.meguerrcy Law field and of spectrum Operativan retentions megueroly	
Anan Automation Receitarie-oue	• Version freedom	0.5atterr	Spectral resolution	
User	LB [H0] = GB = SSB = TM1 =	0.300 0 0 0	Live broadening for en: Gaussian new polition for gen, 0-408+1 Geve twee and 0000 (0.1.2) Left twee for ten 0-47M+1	
	TM2 = Phase correction PHCD (segree) =	-#2.000	Populational flor tro D-TM2+1 Otto order corrections for par	
	PHC1 (Begree) = PH_mol = Therefore corrects	0.000	Fut order correction for prive Privating modes for bit, etc	
	ABSG = ABSF1 (ppm) = ABSF2 (ppm) = BCFW (ppm) = COROFF5 (pq) = DC (ppm) =	8 240.000 -10.000 1.000 0.000 0.000	Despire or perspectrema for pice (D. 5) Left level for interf Depid level for along Piblics width for bio (1990/pib) Connections without for PC_MCO-major with Distances intervals for any status	

b. Fourier Transform:

- Type **efp** in the command line
- c. <u>Phase correction:</u>
 - Manual method
 - Click phase correction \checkmark button in the upper toolbar
 - The Tab bar of the active data window will be replaced by the following toolbar



• Left-click-hold the button and move the mouse until the reference peak is exactly in absorption mode

- Left-click-hold the **1** button and move the mouse until the entire spectrum is exactly in absorption mode
- Click the 🖳 button to save and execute the phase correction



- > Automatic method:
 - Type **apk** in the command line to execute automatic phase correction
- d. Chemical shift calibration
 - Click the button in the upper toolbar, and the Tab bar of the active data window will be replaced by the following toolbar



- Position the red cursor line at the reference peak
- Left-click at that position and enter the chemical shift of the reference peak at the popup dialog box
- e. Integration
- Click the **J** button in the upper toolbar, and the Tab bar of the active data window will be replaced by the following toolbar

HCyclosponn Rouse Sensitivity: 1.0 7.14 ppm / 3568.53 Hz			ada	li	
PERFINE PEOLON MODE Define: Drag using left Return: Left-click high	mouse button				
,-					
. <u> </u>	.lhu	Will	million	WIIWINI.	_
1				2	magi

• Define integral regions: <u>Note: the active button is highlighted in</u> <u>green</u>

- : define integral region interactively
- ط: define integral region via dialog
- H: cut integral region
 - ➤ When this button is highlighted in green, put the red cursor line at one edge of a peak or multiplet, then left-click-hold and drag the cursor line to the other edge of the peak or multiplet.
- > Use $\overset{\triangleleft}{\vdash}$ or $\overset{\triangleleft}{\checkmark}$ buttons to modify the integral region.
- Select a single integral region
 - Right-click in the integral region you want to select
 - Choose Select/Deselect from the popup menu
 - ➡ : select the next integral region
 - : select the previous integral region
 - : select all integrals
 - 🔀 : delete selected integral region from the display
- Calibrate integrals
 - Right-click in the reference integral region
 - Choose Calibrate from the popup menu
 - Enter the desired value for the reference integral and click OK
- Other buttons:
 - *2 /2 🗢 *X
 - : Scale selected integrals
 - \pm **\uparrow \uparrow** : Move all the integrals up and down
 - \square \square : Change the mouse sensitivity
 - /b /s # : Perform interactive Bias and Slope correction
 - ¹: Save integrals and return
 - Leturn, discarding any changes
- f. Peak picking:
 - Click the *button* in the upper toolbar, and the Tab bar of the active data window will be replaced by a following toolbar



• Define peak picking regions: Note: the active button is highlighted in green

H: Define peak picking range

- : Change peak picking range
- ★ : delete all peak picking regions

When the button is green, put the cursor at the upper-left corner of a peak picking range, then left-click-hold and drag the cursor to

the low-right corner of the range. You can use this utton to modify the peak picking range.

- Other buttons in the toolbar
 - : Define peaks manually
 - : Define peaks semi-automatically
 - [™]: Delete all peaks
 - Example: Save the peak region and peak list and return
 - + : Return, discarding any changes

8. How to process a 2D NMR spectrum

- a. Fourier transform:
 - Type **xfb** in the command line
- b. Phase correction:
 - Click phase correction \checkmark button in upper toolbar
 - The Tab bar of the active data window will be replaced by a following toolbar



- Right-click and choose **add** in the popup menu to select three peaks at different parts the spectrum
- Click the button to display rows of selected peaks under phase row mode



- Perform phase correction by click-holding the button and
 1 to make all peaks in three rows in absorption mode
- Click the 💾 button to execute, save and return
- Click the button to display columns of selected peaks under phase column mode
- Perform phase correction by click-holding the 0 button and 1 to make all peaks in three rows in absorption mode
- Click the 🖳 button to execute, save and return
- Other buttons in the tool bar

+ - : show next or previous row/column

: arrange row/column horizontally or vertically or vertically in a split window

- Click the J button to return from 2D phase mode
- c. <u>2D chemical shift calibration</u>
 - Click the ^A button in the upper toolbar, and the Tab bar of the active data window will be replaced by the following toolbar



• Left-click at the reference peak in the data window, the dialog box will appear _____

🥌 calibrate	
Spectrum calibratio	n frequency
F2[ppm]	F1(ppm)
3.3168	3.3871
	OK Cancel

- Enter the F2 and F1 chemical shifts you want to assign to the reference peak
- Click ok

9. How to display multiple 1D /2D spectra

a. Click the the button in the upper toolbar, and the Tab bar of the active data window will be replaced by a following toolbar



- b. Add a dataset:
 - Enter **re** and specify the additional dataset
 - **OR** 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
- c. Select/deselect the datasets
 - The browser is split in two parts and in the lower part you can click one dataset to select it
 - **OR** click in the corresponding area in the data window
 - Click the th button to deselect all the datasets
- d. Remove a dataset:
 - Select a dataset you want to remove as step c
 - Click the $\stackrel{\texttt{M}}{\overset{}}$ button to remove it
- e. Other buttons:
 - : Toggle between superimposed and stacked display
 - : Switch on/off display of datapaths and scaling factors
 - \triangle : Show the difference between the first and the sum of the other datasets
 - Σ : Show the sum of all datasets in the multiple display window

10. How to perform multiplet analysis?

- a. Perform Peak-picking as Procedure 7(f) (you might need use manual peakpicking the button to pick all peaks)
- b. In Menu bar, click Analysis \rightarrow Structure Analysis \rightarrow Multiplet Definition [mana]
- c. The Tab bar of the active data window will be replaced by the following toolbar



d. Automatically define multiplet

- Click the the button in toolbar to define multiplet in whole sweep width automatically
- Click the button in toolbar; left-click-hold mouse and drag to define the region, multiplet in this region will be defined automatically.
- e. Manually define multiplet
 - Click the ⁺ button in the toolbar
 - Put red cursor line on a peak and left-click to select, repeat to select other peaks, then right-click and select **Define Multiplet** in the popup menu



- Click the button in the toolbar to couple existing multiplets
 Left-click to select each multiplet
 - Right-click and select Define Multiplet in the popup menu



- The coupling constants will be listed in the up-right corner of the window
- Click the button in the toolbar, the resulting report will show in popup window



f. Click the \blacksquare button in the toolbar, and save multiplet assignment and return

TOPSPIN PLOT EDITOR INSTRUCTIONS

- 1. How to use TOPSPIN PLOT EDITOR to plot a spectrum?
- 2. How to plot several 1D spectra in stack mode in Topspin Plot Editor?
- 3. How to export a spectrum as PDF or PNG or EMF format file so you can insert it to your report/thesis?

1. How to use TOPSPIN Plot Editor to plot a spectrum

a. Type **Layout** in the command line to select the desired layout by clicking downarrow button of LAYOUT box , then type **plot** in the command line and TOPSPIN Plot Editor will start

LAYOUT		×
Layout file for 'auto	plot'	
LAYOUT =	+/1D_X.xwp	*
		OK Cancel

b. OR File→Print, and select Print with layout-start Plot Editor in the popup window

😂 Print [Ctrl+P] , pla	it.	$\mathbf{\times}$
Options		
○ Print active window	[prnt]	
Print with layout - st	tart Plot Editor (plot)	
 Print with layout - p 	lot directly [autoplot]	
Required parameters-		
LAYOUT =	+/1D_H.xwp	
Use plot limits	Fill data set list	
Irom screen / CY	from your default portfolio	
O from Plot Editor Re	set Actions	et
O as saved in Plot Ed		
Override plotter sav	ved in Plot Editor:	
CURPLOT =	hp LaserJet 1300 PS 🛛 🗸	
·	OK Cancel Help	

In the required parameters, select the desired layout by clicking down-arrow button in **LAYOUT** box. After clicking **OK** button, the TOPSPIN Plot Editor will start

The layout can be specified by using one of the following abbreviations:

- +: the standard layout directory: ../topspin/plot/layout
- ~: the user home directory
- #: current processed data directory
- c. Preview the current plot layout and plot (Click File \rightarrow Print)



d. Modify the plot layout

Move, resize and delete an object (spectrum, title, parameter or logo):

- Mark an object by clicking the button and then clicking the object
- Click-hold the object and move the mouse to move the object
- Click-hold one of the green markers and move the mouse to resize the object
- Click the Delete button in command bar to delete the object

Modify the spectrum

• Mark the spectrum object and click the ^{1D/2D-Edit} button in the command bar



Mark the spectrum object and click the Edit button in the command bar



Edit Stack ID Septem Data Stell Basic Unite XAves: P ppm H 2 Points Peak labels: © ppm H 2 Points Peak labels: © ppm H 2 Points Peak labels: © ppm H 2 Points Peak labels: Text Formet X.3 Attributes Integrals: Vinix, Yinax 6.70757=0.09, 1.37063e-011 V Show Integrals X.3 Vinix, Yinax 4.7057e-0.09, 1.37063e-011 V Show Integral Labels Text Format X.2 Attributes Scaling Information for X axis Attributes OK Cancel Apply	Under 1D Spectrum tab, you can modify the units of axes and peak (ppm or Hz), attributes of peak labels and integral labels
---	---

Under Linux, all parts (Graph, 1D spectrum. DataSet and Basic) are shown simultaneously

Edit Display Object	X
1D Spectrum:	1
Show Peaks Show Peak Marks	
🗏 Show Integrals 🖉 Show Integral Labels	
Labels above X axis	
Peaks Text Format: [%.3f	
Integrals Text Format: [%.2f	
Integral Ymin, Ymax: 9.43388e+09 , 1.96496e+11	
Units for X-Axes: \diamond ppm \diamond Hz \diamond Points	
Units for Peak Labels: \diamondsuit ppm \diamondsuit Hz \diamondsuit Points	
Attributes: Peaks Integrals Scaling Info	
Basic NMR:	
Data Set: Select from Portfolio	_
ki j	Ε. Γ
OK Apply Cancel	

If the spectrum is a 2D spectrum, the popup window is

aph 20 Spectrum 20 Pr	piections Data	Set Basic
Data Sets		
🔽 Top Size	3.00	Select
F Bottom Size	2.00	Select
Left Size	2.00	Select
ERight Size	2.00	Select
Attributes		

Under **2D Projections** tab, you can define the projections on F1 (left/right) and F2 (top/bottom) dimensions from 1D datasets Modify parameters and title

• Right-click the object and choose corresponding buttons in the popup menu to modify the object

2. How to plot several 1D spectra in stack mode in Topspin Plot Editor

a. Click the **Data** button in the command bar, click **Edit** button in the popup **Data Set Selector** window. The **Portfolio Editor** window will pop up

Data Set Selector	X	Partiala Editor			8
1: C/Binker/TOPSPNI/data/guest/min/exam1d_192/1/pdat	OK Apply Cancel	Directory Construction Construction Construction Director	Name: ITEC/1124 EXECUTION EXEC	Expro:	Process
X	Edit Set	Ponendaz [C:20:udurer/YOPSP92/3data/guerec/rem Apply	r/examild_132/1/pdala/1	Remove	1

- b. In **Portfolio Editor** window, choose right **Directory** and **User**, all datasets will show up.
- c. Choose the first spectrum by clicking the respective entries in the sections **Name**, **Expno** and **Procno**. Then click the **Append** button.
- d. Repeat step **c** for the rest of spectra, then click **Apply** back to **Data Set Selector** window, click **OK**
- e. In **TOPSPIN Plot Editor**, click **File** \rightarrow **New** to open a new layout
- f. Click the button, click-hold left mouse button and drag in the layout area



g. Mark the spectrum by click the button, then click Edit button in command bar. The popup window is

lingen (1D Specif	tas Stecked [C	ana tanj Barm	
Reambur of Shack	nd Spectra 👔		
Specific Officet	F	0.0 + 0.2	

h. Click **Stacked** menu bar, fill the box. In Spectra Offset box, the first number is offset of X-axes, and the second number is offset of Y-axes. By adjusting these two offsets, you will get the desired layout

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	1	1	.1	in the state of the

- **3.** How to export a spectrum as PDF or PNG or EMF format file so you can insert it to your report/thesis?
 - a. From Topspin Plot Editor
 - A spectrum is appeared in the Plot Editor with desired layout
 - Click **File** → **Export**

Seen	My Documents	+ 🕲 🗗 🖽 -	
My Rocard Documents Decklags My Disconnets My Computer	Mr Hauk Mr Hauk Mr Houres Mr Houres Mr Houres Mr Josef Mr Josef Mr Josef Mr Josef Mr Shares Mr Shares		

• In the box of **Save as type**, you can choose the type you want, and put filename in box of **File name**, then click **Save** button

b. From Topspin (Note: No PDF type is available)

- A spectrum is appeared in the data area
- Click **File** → **Export**

Look m	La Amôu	
My Recent Documents Desitop Desitop Desitop My Documents My Composer My Network Places	tangen (HPAH 60 1205446 Appen (Mon Charles Cartests Cartests Cartests Develop Model (Mon Charles) Sendfo Statt News Tempates	
	Faroure	- Finan

- Put filename in the **File name** box with extension
- Click **Export** button