

UNIVERSITE CATHOLIQUE DE LOUVAIN

GROUPE DE RMN



VERSION 1.1

by Dr David Chapon -21/06/06

1. Display Description

 \succ The menu line

File Edit View Processing Analysis Options Window Help

➤ Two icon lines

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 \succ The browser



 \succ The spectral window



 \succ The command line

2. 1D Experiment Processing

- Open your spectrum by double clicking on its name in the browser window or dragging it from the browser to the spectral window.
- Check the processing parameters in the process parameter window (ProcPars menu) before doing the Fourier transform of the signal.

Test 10 1 C:\Bri	uker\TOPSPIN Chapon						
Spectrum Proc	Pars AcquPars Title	PulseProg Peaks Integra	Is Sample Structure Fid				
ы S 🖽 🗛							
Reference	Deference			^			
Window	SI =	32768	Size of real spectrum				
Phase	SF (MHz) =	500,1999723	Spectrometer frequency				
Baseline	OFFSET (ppm) =	11.063	Low field limit of spectrum				
Fourier	SR [Hz] =	-27.70	Spectrum reference frequency				
Integration	HZpPT [Hz] =	0.183399	Spectral resolution				
Peak	Window function			=			
Automation	WDW =	EM	Window functions for trf, xfb,				
Vilscellarieuus	LB [Hz] =	0.30	Line broadening for em				
0361	GB =	0	Gaussian max. position for gm 0 <gb<1< td=""><td></td></gb<1<>				
	SSB =	0	Sine bell shift SSB (0,1,2,)				
	TM1 =	0	Left limit for tm 0 <tm1<1< td=""><td></td></tm1<1<>				
	TM2 =	0	Right limit for tm 0 <tm2<1< td=""><td></td></tm2<1<>				
	Phase correction						
	PHC0 [degree] =	-184.684	Oth order correction for pk				
	PHC1 [degree] =	0.055	1st order correction for pk				
	PH_mod =	no 💌	Phasing modes for trf, xfb,				
	Baseline correction						
	ABSG =	5	Degree of polynomial for abs (05)				
	ABSF1 [ppm] =	240.000	Left limit for absf				
	ABSF2 [ppm] =	-10.000	Right limit for absf				
	BCFW [ppm] =	1.000	Filter width for bc (sfil/qfil)				
	COROFFS [Hz] =	0.00	Correction offset for BC_MOD=spol etc.				
	BC_mod =	quad 🕑	Fid baseline modes for em, ft, xfb,				
	Fourier transform						
	TDeff =	0	# of fid data points used by ft				
	STSR =	0	First output point of strip transform				
	STSI =	0	Total # of output points of strip transform				
	ME_mod =	no 💌	Linear prediction for ft, xfb,				
	NCOEF =	0	# of LP coefficients				
	I PRIN =	0	# of output points for LP	×			

Essential processing parameters for 1D treatment

SI: Number of points in the frequency domain. If SI > TD/2, the FID is zero filled (TD: Number of points in the acquisition time domain: AcquPars menu).
SR: Spectrum reference. Parameter to report in each 1D spectrum to calibrate them in the same way (the spectrum calibration is correlated to this parameter).

WDW: Choose EM to apply an exponential multiplication to your FID.
LB: Factor of line broadening for EM. Enter 0.3 as standard for ¹H and 2.0 for ¹³C.

Click on Process 1D in the icon line to do a Fourier transformation, an automatic phasing and a baseline correction.

1. Phase Correction

➤ If the phase is not correct, phase the spectrum manually by clicking on I icon. You will move in the following window.



The red cursor on the spectrum is the pivot point for the first order phase (by default the biggest signal). If you want to change this pivot point put the black cursor on another signal. Click right with the mouse, and select Set Pivot Point.



- Phase to zero and first orders by keeping clicking the mouse left button respectively on the two icons
 (zero order) and
 (first order) and moving the mouse vertically.
- ➤ When the spectrum is correctly phased click on ↓ to save the phase and return to the classical spectral window.

2. <u>Calibration</u>

Do an expansion of the signal you want to calibrate by keeping clicking the mouse left button and moving the mouse from one side to the other side of the selected signal (with icon activated).



Calibrate the spectrum by clicking on in the following window.

	Test 10 1 C:Bruker/TOPSPIN Chapon	
-28	لر <mark>ا</mark>	• •
10 1401	<pre> Crotonale, 13C, CDC13, Tamb, Pauli le 26/04/06 -7.2876 ppm / 3645.2329 Hz / 500.20361753 MHz / Index = 10297 - 10298 pefine Reference FREQUENCY pefine Reference FREQUENCY pefine Left-click inside data window </pre>	
u		
с 4		
	7.6 7.5 7.4 7.3 7.2 7.1	[ppm]

- Put the red cursor on the top of the signal you want to calibrate and click left.
- > The following window appears.



Enter the new value of chemical shift (in ppm) and click on OK.
You will automatically quit this calibration window.

icon. You will move

3. <u>Baseline Correction</u>

You can click on icon to do a specific baseline correction. The easiest way is to enter 'abs' in the command line, it will do a classical baseline correction + automatic integration of the main patterns. You could change the integration of these patterns in the integration mode. Enter 'abs n' in the command line to do only a baseline correction without integration.

4. <u>Peak Picking</u>

Click on icon to enter the peak picking routine. It will open the following window.



 \succ The icon $\stackrel{\frown}{\longrightarrow}$ is activated by default.

On the signals you want to peak pick, draw a green region with the mouse (by keeping clicking the left button of the mouse) as in the following window. For each selected region the peak picking appears in red at the top of the window.



- You can expand the selected regions by activating the icon, and move the limits of each green region with the mouse.
- ➤ You can delete the peak picking or the selected regions by clicking respectively on or icon.
- When you have finished with the peak picking click on icon to save it and return to the spectral window.

5. Integration

Click on icon to enter the integration routine. It will display the following window.



- If you have some integrals displayed, there are those obtained before with the 'abs' command. If you want to delete them: First click on icon to select all the integrals (all the integrals labels are then coloured in green) and click on icon to delete them. It will ask you whether you are sure to delete all the integrals: Click on OK.
- Click on icon to do a manual integration (it is activated when it is green).
- Create your integral by keeping clicking the left button of the mouse and move the mouse from one side to the other side of the signal you want to integrate as in the following window.



- > The first integral defined takes by default the value 1.
- Proceed with all your signals in the same way.
- ➤ To calibrate one integral put the cursor under it, click right and select the line Calibrate.

Test 10 1 C:Bruker/TOPSPIN Chapon	
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Crotonate, 13C, CDC/3, Tamb, Pauli le 26/04/06 Mouse Sensitivity: 1.0 1.18 ppm / 592.41 Hz DEFINE REGION MODE DEFINE REGION MODE DEFINE: Drag using left mouse button Return: Left-click highlighted icon	
	Select / Deselect
6	Calibrate Normalize Lastscal Delete
	[mqq]

 \succ In the open window, enter the new value of your integral, and



If you want to delete one integral, put your cursor under it, click right and select Delete.



- If you want to adjust the slope or the bias of one integral, select it by a right click with the cursor under the integral. When it is selected the integral value is coloured in green. Change the slope and the bias by keeping clicking the mouse left button respectively on the icon 1/s and 1/b and moving the mouse vertically.
- When you have finished with the integration click on icon to save it and return to the spectral window.

6. <u>Printing</u>

Display in the spectral window what you want to print. Thus click right in the spectral window and select Display Properties.



Select the parameters you want to display on the following

window.

🔄 . dopt	
Please select the components to together with the spectrum (if av	o be displayed /ailable):
Cursor information	
Title	
Status parameters	
Integrals	
Integral labels	
Peak labels	
Multiplets	
Show data points	
OK OK	Cancel

When you have all your desired parameters on the spectral window, click on to print. The following window appears.

 Options Print active window (prnt) (m) Print with layout - start Plot Print with layout - plot directly 	litor (plot) (autoplot)
Required parameters	
LAYOUT =	~
Use plot limits	Fill data set list
from screen / CY from Plot Editor Reset Actions	O from your default portfolio
as saved in Plot Editor	from portfolio saved in data se

> Select Print active window, the following window appears.

Printer			
Name:	HP Business Inkjet 2800 PCL 6	Properties	
Status:	Ready	4	
Туре:	HP Business Inkjet 2800 PCL 6		
Where:	IP_130.104.26.27		
Comment	:	Print to file	
Print rang All Page C Selec	e s from: 1 to: 9999 tion	Copies Number of copies: 1 = 1 1 2 3 Colla	• •
		OK Cance	el l

 \blacktriangleright Select your printer and click on \overline{OK} .

> The following window appears.

	Demonstrational data Demonstrational data Demonstrational processing Demonstrational processing Demonstrational processing	
	P House H Signer Phononemianian P A definition of the second s	
	Prova Proving Phenomenanian Conference on Phenomenanian Proving Ph	
Paper		
Size: 🗛		
Server Ea	rm Select	•
Jource. jru		
Orientation	Margins (inches)	
Orientation	Margins (inches)	1
Orientation C Portrait C Landscape	Margins (inches)	1

Select the size of your desired paper (A3 or A4), and click on OK.

3. 2D Experiment Processing

- Open your spectrum by double clicking on its name in the browser window or dragging it from the browser to the spectral window.
- Check the processing parameters in the process parameter window (ProcPars menu) before doing the Fourier transform of the signal.

Test 11 1 C:\Bri	uker\TOPSPIN Chapon				
Spectrum Proc	Pars AcquPars Title	PulseProg Peaks I	ntegrals Sample	Structure Fid	
OS 123 AA					
Reference		ED	E1	Frequency avia	
Vindow	Deference	12	1.1	Trequency axis	
hase	SI =	2048	512	Size of real spectrum	
aseline	SF [MHz] =	500,1999723	500.1999723	Spectrometer frequency	
ourier	OFFSET (ppm) =	11.063	11,108	Low field limit of spectrum	
eak	SR [Hz] =	-27.70	-27.70	Spectrum reference frequency	
utomation	HZpPT [Hz] =	2.934382	11.826370	Spectral resolution	
iscellaneous	Window function	Leves			
ser	WDW =	SINE	SINE	Window functions for trf, xfb,	
	LB [Hz] =	0.30	0.30	Line broadening for em	
	GB =	0	0.1	Gaussian max. position for gm 0 <gb<1< td=""><td></td></gb<1<>	
	SSB =	0	0	Sine bell shift SSB (0,1,2,)	
	TM1 =	0	0.1	Left limit for tm 0 <tm1<1< td=""><td></td></tm1<1<>	
	TM2 =	0	0.9	Right limit for tm 0 <tm2<1< td=""><td></td></tm2<1<>	
	Phase correction				
	PHC0 (degree) =	-162.716	0.000	Oth order correction for pk	
	PHC1 [degree] =	0.000	0.000	1st order correction for pk	
	PH_mod =	no 💙	mc 💌	Phasing modes for trf, xfb,	
	Baseline correction				
	ABSG =	5	5	Degree of polynomial for abs (05)	
	ABSF1 [ppm] =	240.000	1000.000	Left limit for absf	
	ABSF2 [ppm] =	-10.000	-1000.000	Right limit for absf	
	BCFW [ppm] =	1.000	1.000	Filter width for bc (sfil/qfil)	
	COROFFS [Hz] =	0.00	0.00	Correction offset for BC_MOD=spol etc.	
	BC_mod =	quad 😪	no 🖌	Fid baseline modes for em, ft, xfb,	
	Fourier transform				
	TDeff =	0	0	# of fid data points used by ft	
	STSR =	0	0	First output point of strip transform	
	STSI =	0	0	Total # of output points of strip transform	
	ME_mod =	no 👱	no 💌	Linear prediction for ft, xfb,	
	NCOFF =	10	10	# of LP coefficients	

Essential processing parameters for 2D treatment
SI (F1/F2): Number of points in the frequency domain. For each dimension, if SI > TD/2, the FID is zero filled (TD: Number of points in the F1/F2 time domain: AcquPars menu).

• SR: Spectrum reference. Put the same value of 1D spectrum to calibrate each dimension of the 2D experiment as the 1D experiments.

- WDW: Choose EM to apply an exponential multiplication to your FID.
- LB: Factor of line broadening for EM. Enter 0.3 as standard for ¹H and 2.0 for ¹³C channel.
 - Click on Process 2D in the icon line to do Fourier transforming.
 You will have the following display in the spectral window.



Add the correct 1D external projections on each side of the 2D by clicking right on a 1D projection, and select External Projection.



> Fill the following window with the user, the name and the experiment number of the 1D experiment, and click on \overline{OK} .

Options							
Oisplay data in same window							
O Display data in new window							
NAME =	Test						
EXPNO =	10						
PROCNO =	1						
DIR =	D:\Bruker\TOPSPIN						
USER =	Chapon						



➤ It will display the select 1D spectrum as in the following window.

Proceed with the second dimension in the same way.

To do an expansion on the 2D spectrum, keep clicking the mouse left button and draw a square from one corner to its opposite as in the following example.



Stop keeping clicking the mouse button, and your expansion automatically appears.



➤ To print, display what you want on the spectral window and proceed as with a 1D experiment (see p.12)

4. Superposition of several spectra

With a first spectrum opened in the spectral window, click on tion to enter the multiple display menu. You will obtain the following window on the screen.



Select the second spectrum you want to display in the browser and double click on the experiment number or drag it in the spectral window; it will automatically appear in red in the spectral window and in the multiple display window.



Select one of the spectra in the multiple display window.



- On the first icons line of the spectral window, move up or down the selected spectrum by keeping clicking the ts icon with the left button of the mouse and move the mouse vertically.
- You can increase/decrease the intensity of the selected spectrum or both by selecting your spectra in the multiple display window and click on ²2₅ ¹2₅ icon.



- In the same way, click on sicon to move the selected spectra horizontally.
- > Click on \triangle or Σ icons to respectively do the difference or the sum of the two spectra.
- You will find in the following window the details of the rest of the most interesting icons:



You can now add a third spectrum by processing it in the same way.

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