TOPSPIN - data **processing**

○-🗀 nmrafd open Folder to see file-names
○-🗀 2103yourname open Folder to see all your measurements
drag file in display

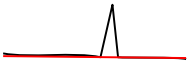
**1H processing**

ef transformation
ap automatic phasing

phasing-manually

 put cursor in “0” or “1” depress mouse and adjust phase
save↵

expand reference-peak (drag to expand)

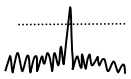
 indicate peak (left click) enter ppm-value  

bn baseline correction is better for integrals

integrate-manually

∫ click  green to integrate , (click  blanc to expand)
drag to integrate (red lines)
if the slope is not good: $\int_b$ interactive bias correction.
integral-calibration right-click in an integral - Calibrate current integral -enter value -ok
save↵

Peak picking:
ppf gives peaks of Full spectrum pps give peaks of Displayed part of spectrum
see if peaks of interest are shown,

>mi minimum intensity (standard value =0.2) mi 
If too many peaks: mi higher (e.g. 0.5) and again ppf
If small peak of interest is not shown: mi lower (e.g. 0.01) and again ppf
( to get small peaks cy=100 , mi=0.01 , pc=0.5 )

 easy define ppm range

xw plot
click green dots and indicate (click) spectrum
Edit -Xmin, Xmax to enter ppm-range , (e.g. 8, -0.1) , ok

1D,2D-Edit

⬍ adjust amplitude
click Expand draw red box for expanding range

File -print -print
close -Plot-editor **ok** close and discard all changes

**Cosy processing**

Put the cosy file in Topspin-display

xfb 2D-transformation (or: x (xfb , levcalc ) )
sym symmetrization

right-click in the top-projection – external projection setproj set projections
check or change expno
ok
right-click in the left projection – external projection
check expno
ok

referencing by use of sr

re 1 (read expno 1 ) (if this spectrum is calibrated)
sr ↵ ctl-c (copy: this value) enter
re 2 (read cosy expno 2 )
sr ↵ ctl-v tab ctl-v (paste: this value, tab , paste this value again)

xw plot
expand draw red box to expand
green dots (click) indicate (click) spectrum

1D/2D-Edit
upper symbols for 2D

⬍ adjust amplitude of 2D
lower symbols is for Top or Left projection

⬍ adjust amplitude of top/left-projection

close-1D/2D-edit

File print print

Close-plot-editor , **Ok** (close and discard all changes)

**13C processing**

ef Fourier transformation
ap automatic phasing manual phasing click 
put cursor in “0” or “1” and move mouse to adjust phase
save↵


expand reference peak
indicate peak left click enter ppm value e.g. CDCl3=77.16 ppm
for D2O sr= -4.35

ppf peaklist
see if peaklist includes smallest-peak-of-interest
if there are too many peaks >mi put in higher value , (see scale for best value)
>ppf new peaklist

e easy define ppm range

xw
green dots select spectrum
1D/2D-Edit
↑ click to fit top inside scale
↓ click " bottom "
or change amplitude

File -print -print
close Plot-editor
ok close and discard all changes

**Noesy - Processing**

xfb (2D-transformation) (or: x (xfb , levcalc ) )
setproj
check projections , right-click in top-projection, external projection , check or change expno , ok
, right-click in left-projection , external projection , check or change expno , ok

referencing by use of sr

re 1 (read expno 1 ) (if this spectrum is calibrated)
sr ↵ ctl-c (copy) enter
re 3 (read Noesy expno 3 )
sr ↵ ctl-v tab ctl-v (paste , tab , paste)

Phasing
click 

select peaks , right-click , add
click **R** to phase rows
adjust phasing with **0** and **1**
save↵

click C to phase columns
adjust phasing with **0** and **1**
save↵

referencing and plot same as cosy.

**HSQC - Processing**

xfb (2D-transformation) (or: x (xfb , levcalc ) )
(setproj)
check projections , right-click in **top**-projection, external projection , check or change **expno 1H**, ok
, right-click in **left**-projection , external projection , check or change **expno 13C**, ok

referencing by use of **sr** values

re 1 (read **1H**-spectrum expno 1 ) (spectrum must be calibrated)
sr ↵ ctl-c (copy) , enter
re 3 (read hsqc expno 3 )
sr ↵ ctl-v (paste) , ↵ sr (**F2** , F1)

re 2 (read **13C**-spectrum expno 2 ) (spectrum must be calibrated)
sr↵ ctl-c (copy) , enter
re 3 (read hsqc expno 3)
sr ↵ tab , (move to F1 position) , ctl-v , ↵ sr(F2 , **F1**)

Phasing
click 
select peaks , right-click , add
click **R** to phase rows
adjust phasing with **0** and **1**
save

click **C** to phase columns
adjust phasing with **0** and **1**
save
↵

xw xwinplot
expand draw red box to expand
green dots (click) indicate (click) spectrum

1D/2D-Edit
upper symbols for 2D

⬍ adjust amplitude of 2D
lower symbols is for Top or Left projection

⬍ adjust amplitude of top/left-projection

close-1D/2D-edit

File print print

Close-plot-editor
Ok (close and discard all changes)