# 2D Data Processing/Display

## Very Easy Processing:

1) Run process macro:
processcosy
processroesy
processhsqc
processhmbc
processhmbc61c
processtocsy

## Easy Processing:

1) Set weighting functions, linear prediction, display parameters and process data for gCOSY or gHMBC61c type:
setLP1 sqsinebell wft2d trace='f2' f full dp10

for gHMBC VNMRJ4.2:
setLP1 sqsineF2-sqcosineF1 wft2da trace='f2' f full dpn10

for anything else type:
setLP1 sqcosine wft2da trace='f2' f full dpn10

for COSY to make data symmetric type:
foldt

2) Print Data
Click on Autoplot button
or
plcosy(10,1.2,1)
if you have a 1D in experiment 1

## Detailed Description of Processing:

1) Fourier transform 1st fid (where t1 time = initial value)
type:
wft(1)

Alternatively, Fourier transform all fids
type:
wft

2) Set linear prediction parameters if desired in t1 dimension
type:
setLP1

3) Set zero filling parameters in F2 and F1 dimensions
[note that setLP1 command will change fn and fn1]
vnmr parameters:
fn and fn1
fn = np (minimum) or 2*np (maybe slightly sharper, but slower processing) or 4*np (very slightly sharper, much slower to process)
fn1 = 2*ni (minimum) or 4*ni (slightly sharper) or fn (for square processed data matrix, required for foldt command in COSY/gCOSY)

4) Adjust weighting functions in t2 dimension
for easy initial adjustment:
for broader lines but less streaking across spectrum in gCOSY/COSY/gHMBC61c type:
sqsinebell

for sharper lines but possibly more streaking in gCOSY/COSY/gHMBC61c type:
sinebell

for broader lines but less streaking across spectrum in any other experiment (so gHSQC, gHMQC, ROESY, NOESY, TOCSY...) type:
sqcosine

for sharper lines but possibly more streaking in spectrum in any other experiment (so gHSQC, gHMQC, ROESY, NOESY, TOCSY...) type:
cosine

for even broader lines than with sqcosine but even less streaking (normally applicable to ROESY/NOESY), type:
cosineroesy

[note that the sinebell macro creates a perfect sine function in both dimensions by setting sb = at/2 and sbs = 'n', sb1 = ni/(sw1*2) and sbs1 = 'n'; the sqsinebell macro creates a sinebell squared function in both dimensions by setting sb = -at/2 and sbs = 'n', sb1 = -ni/(sw1*2 and sbs1 = 'n'; the cosine creates a perfect cosine function in both dimensions by setting sb = at and sbs = -at, sb1 = ni/(sw1) and sbs1 = -sb1; the sqcosine macro creates a cosine squared function in both dimensions by setting sb = -at and sbs = -at, sb1 = -ni/2 and sbs1 = sb1; the cosineroesy macro uses a cosine squared function in both dimensions and additional gaussian function.]

if you would like to do interactive weighting function adjustment type:
wti

[or vnmr menu button:
Adj Weighting]

5) Fourier transform 1st fid again
type:
wft(1)

6) Adjust phase for SOME experiments (TOCSY, NOESY, ROESY), NOT gCOSY nor gHMBC, nor gHSQC. Usually manually phase, be sure that neither the rp nor lp parameters (right and left phase corrects) are greater than +/- 360 after phasing, otherwise there will be a baseline roll. It is preferable to have lp as close to 0 as possible.

7) For baseline correction, set level/tilt (for dc baseline correction) or integral resets points (for bc baseline correction)
vnmr menu:
lvl/tlt
Then set lvl/tlt appropriately as in 1D
then type:
dc (drift correct)

or
Part Integral then Resets
then set Resets points where there are no signals.
type:
bc
Note whether either dc or bc improves baseline.

8) Fourier transform complete F2 dimension (you could transform full 2d at this point if you do not wish to further adjust weighting functions)
for gCOSY or gHMBC type:
wft1d
for anything else type:
wft1da
[or vnmr menu button:
Transform F2]

9) Adjust weighting functions in t1
If you used any of the above macros for weighting function adjustment, the weighting function in t1 is already set, so you may not need to check it.
for interactive weighting adjustment type:
wti

[or vnmr menu button:
Adj Weighting]

10) Fourier transform full 2d
for gCOSY or gHMBC61c type:
wft2d

for any other experiment type:
wft2da
[vnmr menu button:
Full transform]

11) Display full 2d across the whole screen with the F2 dimension as the x-axis in a contour plot:
type:
f full trace='f2' dpn10
f displays the full sw and sw1
full displays across the full screen [it adjusts wc (width of chart),sc (start of chart), wc1 (width of chart in t1), and sc1 (start of chart in t1)]
trace = 'f2' makes the F2 dimension the x-axis (trace = 'f1' would make F1 the x-axis)
dpn10 displays a contour plot with 10 positive contours and 10 negative contours

12) Phase F2 dimension if necessary (cannot phase gHMBC or gCOSY)
The dimension on the x-axis is allowed to be phased in 2D.
Find peak to phase (usually on the left side of the spectrum)
Put cursor on peak and display 1D slice across spectrum
display spectrum type:
ds

Manually, phase as in 1D, you should try not to adjust the lp parameter (left phase correct) much

If there is an error at this point that says cannot phase this data, type:
pmode='full' wft2da ds
Then try phasing again

Redraw 2D, so type:
dpn10

13) Rephase F1 dimension if necessary (should not normally be required)
The dimension on the x-axis is allowed to be phased in 2D.
type:
trace =’f1'
Find peak to phase

Put cursor on peak and display 1D slice across spectrum
type:
ds

Manually, phase as in 1D (do not adjust lp1 at all, lp1 should = 0)
If there is an error at this point that says cannot phase this data, type:
pmode='full' wft2da ds
Then try phasing again

Redraw 2D, so type:
dpn10

14) Reset F2 x-axis if necessary
type:
trace = ‘f2'

15) Display as contour plot
type:
dpn10

alternatively for only positive peaks type:
dp10

for only negative peaks type:
n10

or to change the number of contours enter the full command:
dconi(‘dpcon’,'pos',10,1.2)
where pos = positive (neg is negative or nothing so dconi('dpcon',10,1.2) is both)
10 = number of contours
1.2 = multiplication factor for spacing between contours (it is empirical what is best a number between 1.1 and 1.5 is generally optimal)

16) Baseline correct if necessary (only on TOCSY or ROESY or NOESY, never on any of the others)
first try drift correct based upon lvl/tilt
type:
dc2d(‘f2')

if that looks good, continue, if that looks worse, must reprocess 2D, so wft2da

then try baseline correction based upon integral resets
bc(‘f2',0)

if that looks good continue, if that looks worse, must reprocess 2D, so wft2da (or change the Resets points and try the bc command again)

17) Make data symmetrical if necessary and possible (sometimes good for gCOSY, does not work for almost any other data set)
type:
foldt

18) Reference Spectrum
rl(Xp) for F2 dimension
rl1(Xp) for F1 dimension
where X is the chemical shift value
if F1 is 13C, then rl1(Xd) not (Xp); if F1 is 15N and 15N is on 3rd channel, then rl1(X*dfrq2)

19) Adjust vertical scale
vnmr parameter:
vs2d

Can used vnmr menu button:
vs +20%
vs -20%

Also, can manually type in value, such as
vs2d=200

Or can use mathematical functions:
vs2d=vs2d*2
that would set the vertical scale to twice its current value

Or can use middle mouse button,
Click on the spot is the appropriate amount of noise

20) Plotting
for full rectangle plot (both positive and negative contours) type:
pn10
for full rectangle plot (positive contours only) type:
p10
for full rectangle plot (negative contours only) type:
n10

to change the number of contours, use full command type:

pcon(15,1.3) page
for a spectrum with 15 contours and a spacing factor of 1.3

for square plot with 1Ds on the side type:
plcosy(10,1.2,1)
where 10 is the number of contours, 1.2 is a spacing factor between contours and 1 is the experiment number with the proton experiment (so if your experiment with the proton was exp3 it would be plcosy(10,1.2,3)

for square plot of 1H/13C correlation with 1Ds on the side if you have both 1H and 13C 1Ds type:
plhxcor(10,1.2,1,2)
where 10 is the number of contours, 1.2 is a spacing factor between contours and 1 is the experiment number with the proton experiment and 2 is the experiment number with the carbon experiment

for rectangle plot with 1D slices on the side,
adjust screen width of 2D with wc and wc1 parameters (width of chart and width of chart in t1), click on menu button:
Proj
then menu button:
Horizontal Proj Max
then adjust vertical scale on 1D
then menu button:
Plot
then menu button:
Vertical Proj Max
then adjust vertical scale on 1D
then menu button:
Plot
then plot 2d with any of the p10, pn10, n10, or pcon(10,1.2) page commands