

Basic 2D NMR and List of Useful 2D VNMR Commands

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This preliminary list includes useful VNMR commands, macros and IU macros. It does not include most parameters. Help on most of these commands can be obtained with `man('command')`, example: `man('pcon')`.

2D NMR Setup/Acquisition Guide

- Our goal for routine 2D NMR is that you be able to set the experiments up in one step, either by typing in the macro name or selecting the experiment from the Setup / Other/2D menu, then process them in one step by typing in the appropriate processing macro name or again selecting it from the Process / Other/2D menu. You will sometimes want to modify this process to achieve desired results.

- Although not necessary, you will usually want to start with an optimized 1D spectrum. Minimally use `movesw` to get the desired expansion and phase it. You will also usually want to move the parameters to another experiment (example: `mp(1,2)`) then run a 2D setup macro to convert the 1D parameters to the desired 2D parameters.

- The setup macro name for the desired experiment can be typed in directly (example: "iugdqcocy") or selected from the 2D/Other menu. Current macro names are listed below.

- To check initial parameters for most 2D experiments obtain just the first increment of a 2D data set by setting `ni=1` and `phase=1` (if phase sensitive). This will not work for echo type experiments such as `dqcocy` where the first increment should contain no signal.

- To increase or decrease the time a 2D experiment will take - vary `ni`, `nt` and possibly `d1`. As a rough guide `d1` should usually be 1-1.5 seconds. `ni` needs to be minimally 64 or better yet 96, and rarely greater than 200. `nt` requirements vary depending on the experiment. In general gradient experiments will require `nt` to be a multiple of 4, but for some such as `gCOSY` `nt` can be 1. For non-gradient experiments `nt` will usually need to be a multiple of 4 or 8.

- By convention the first dimension of a 2D spectrum is called F2 and the second dimension ("increments" as related to `ni`) is called F1.

SEE "**List of Useful 1D VNMR Commands**" FOR MORE on SETUP/ACQUISITION

Current 2D Setup Macro Names (I400 and I500)

iucigar, iucocy, iudqcocy, iugcocy, iugdqcocy, iughmqc, iughsqc, iuhmbc, iuhmqc, iuhsqc, iunoesy, iuroesy, iutocsy

2D NMR Processing

`gaussian` – sets gaussian window function in F2, for F1 use `gaussian('f1')`

`iucosyproc` – automated processing for cosy and gcocy experiments

iudqcosyproc – automated processing for dgcosy and gdqcosy experiments
iuhmbcproc – automated processing for hmbc and CIGAR experiments
iuhmqcproc – automated processing for hmqc, hsqc, ghmqc and ghsqc experiments
iunoesyproc – automated processing for noesy, roesy and tocsy experiments
lp2d(points) – set up linear prediction in F1, can be specified as: lp2d(512)
pmode – use pmode='full' to be able to phase second dimension (F1)
sinebell - sets sinebell window function in F2, for F1 use sinebell('f1')
wft1da - standard half transform (F2 only) if phase=1,2 (phase sensitive)
wft1d - standard half transform (F2 only) if phase=0 or 1 (absolute value)
wft2da - standard 2D Fourier transform if phase=1,2
wft2d - standard 2D Fourier transform if phase=0 or 1 or does not exist
wtia – interactive window function display for the active dimension ("trace")

wft1da and wft2da use flcoef if it exists

2D NMR Display

For display and plotting the active dimension is set with trace = 'f1' or 'f2' and will be the dimension shown horizontally.

abc – auto baseline correct in the active dimension
dconi – display 2D image map for 2D NMR
dpcon/dpconi – display 2D contour map for 2D NMR
mark – put cursors around a peak and type mark to get the peak volume
proj(exp) – puts 1D skyline projection of active dimension in another experiment, proj(8)
r(n) – recall display parameter set saved with s(n)
rl(shift) – set F2 reference on the cursor location, example: rl(7.26p). Note: rl and rl1 function as described regardless of what the active dimension is
rl1(shift) – set F1 reference on the cursor location, typically use as: rl1(77.0d)
s(n) – save display parameters, s1-s9 can be used, recall with r(n)
trace - parameter to change active dimension, trace='f1' or 'f2'
vs2d – 2D vertical scale parameter, can be adjusted for example as vs2d=vs2d*3
zoom – interactively enter limits for expansions

2D NMR Plotting

To preview contour plots use dpcon, which is affected by the th parameter unlike dconi.

iuplcosy – plot homonuclear 2D spectra, see man('iuplcosy')
iuplhxcor – plot heteronuclear 2D spectra, see man('iuplhxcor')
pcon – the basic 2D plotting command
plot2d – general purpose interactive 2D NMR plotting routine, see man('plot2d') – try this one first