List of Commands and Parameters

For information about a command or parameter, in VNMR top window, type:
man('parameter_name')
the information will display in bottom text window

Below are a list of commands and parameters organized in a format that breaks them down into what they do. These are the categories:

1) Commands that directly communicate with the console

2) Standard 1D Acquisition parameters

3) Commands to adjust spectral width/center of spectrum

4) Standard 1D Processing Parameters

5) Weighting Function

6) Linear Prediction

7) Integration/Baseline Correction

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Commands that directly communicate with the console:

acqi
open acquisition window (lock/shim window); acquisition window can normally be opened with Acqi button on right side of top menu bar

su
setup; setup parameters, communicates with console; required to tune probe, change temperature, read and load shim file

go
acquire data

ga
acquire data and process with wft command (processing only takes place after acquisition is finished)

aa
abort acquisition

sa
stop acquistion, acquisition can be restarted with ra

ra
resume acquistion

e
eject sample

i
insert sample

Standard 1D Acquisition parameters:

nt
number of transients (also referred to as number of scans or acquisitions)

bs
block size; amount of scans after which data is written to hard drive, should normally be set equal to the phase cycle, which is 4 for a standard 1D

d1
relaxation delay; delay before first pulse; also called recycle delay

sw
spectral width; also referred to as sweep width; width in Hz of the spectrum; for example a 10 ppm spectral width on a 500 MHz spectrometer would be = 5000 Hz whereas on a 200 MHz spectrometer sw = 2000 Hz; to change sw to 10 ppm type sw = 10p; if only 10 is typed without the p argument then the sw = 10Hz

tof
transmitter offset; center of spectrum for nucleus being detected; tof = 0 is not 0 ppm (tof = 0 is ~5ppm)

solvent
solvent parameter; adjusts referencing and center of spectrum based upon solvent being used

pw
pulse width; the time in microseconds of the pulse for the experiment

tpwr
transmitter power; the power of the pulse used in the experiment

pw90
the approximate value of the 90° pulse at a given power level (tpwr); changing pw90 has no effect on the actual experiment; however, some macros use pw90 to determine proper pulse widths to be used in the experiment

gain
receive gain; the amplification of the signal; higher gain means more amplification (normally gain =’n’ which means that the computer will determine the optimal value)

at
acquisition time; the length of time that the receiver is actually acquiring data; correlated to the digital resolution and the T2* relaxation time

np

number of data points acquired (correlated to the acquisition time and spectral width)

fb
filter bandwidth; the bandwidth in Hz from the center of the spectrum that the receiver will accept; automatically set to 10% more than half of the spectral width

tn
transmitter nucleus, nucleus being detected

sfrq
spectrometer frequency of the nucleus being detected in MHz; the actual frequency being detected is affected by the tof and the solvent parameters

temp
temperature parameter; temp = 30 followed by su will change temperature to 30° C; temp = 'n' followed by su deregulates temperature; temp is a parameter such that probe/sample temperature might be equilibrated at 30, but when a new parameter set is loaded then su or go or ga are typed, temperature will change to new value

vttype
variable temperature type; if vttype = 0, then temperature will not change no matter what the temperature parameter is set to; if vttype = 2 then temperature will change according to temperature parameter

spin
spin rate parameter, spin rate is adjustable in Acqi window, but also can be a parameter like any other; thus, spin = 20 followed by su will set spin rate to 20; normally, spin rate parameter is not used, spin is controlled through Acqi window

dof
decoupler offset; equivalent to tof for decoupler nucleus; as with tof, dof = 0 is not 0 ppm

dn
decoupler nucleus

dfrq
decoupler frequency in MHz

dm
decoupler mode; sets when the decoupler is turned o; for example, dm = 'nnn' means decoupler is set to no for the whole experiment; dm = 'nny' means decoupler is on during timer period 3, usually the acquisition time; dm = 'ynn' means decoupler is on during time period 1, normally the d1 relaxation delay

dmm

decoupler modulation mode; sets type of decoupling used, normally dmm =’www’ for Waltz type decoupling

dpwr
decoupler power; equivalent to tpwr for decoupling, dpwr should almost never be more than 49 units, normally 35-45 units

dmf
decoupler modulation frequency; the dmf is the frequency range that needs to be decoupled in Hz; must correlate to dpwr as 1/dmf = pulse for decoupling

dfrq2
2nd decoupler nucleus frequency (only applies to consoles and probes that have the ability to detect 3 nuclei simultaneously

dmf2, dpwr2, dmm2, dm2 are equivalent for 2nd decoupler nucleus

Commands to adjust spectral width/center of spectrum:

movetof
move transmitter offset; if you put the cursor in a specific spot in the spectrum, and type movetof, the tof will be moved to where the cursor is. Since the tof is an acquisition parameter, movetof only affects the tof (the center of the spectrum) the next time go or ga are typed

movesw
move spectral width; similar to movetof command except now both tof and sw are changed. Set both cursors on edge of spectrum, type movesw and spectrum is now recentered and the sw is reduce to positions of cursors

centersw
put cursor in center of spectrum

Standard 1D Processing Parameters:

ft
Fourier transform, will use linear prediction and zero-filling, does not use weighting function

wft
weighted Fourier transform, does use weighting function

fn
Fourier number; how many points over which FID will be transformed. If fn < np, then data will be cut off at that point of FID; if fn > np, zeroes (0 amplitude) will be added to end of FID, if fn = ‘n’ n zero fill is used; normally should be either set to ‘n’ or between np and 4*np

wti
interactive weighting; brings up display of FID, weighting function being used and result of wft command with that weighting function with real time adjustments. If weighting function is changed, wft must be typed for the weighting function to be accepted

rp = right phase correct; zero order phase correct; should change phasing of spectrum equally across the entire spectrum; during interactive phasing, the first mouse click will lead to adjustment of only rp phase correct; rp normally should not be greater than 360 or less than -360

lp
left phase correct; first order phase correct; will change the right side of the spectrum more than the left side of the spectrum; during interactive phasing, the second (or any successive) mouse click will lead to adjustment of both lp and rp phase corrects; should almost never be greater that 360 or less than -360, and should ~0 ideally

aph
autophase spectrum

Weighting Function:

lb = line broadening; weighting function that will approximately add the value of lb to the width of resonances in Hz. Thus, if the line width at half-height is 0.2 Hz and lb = 1 then that resonance will have line width of 1.2 Hz after wft command. lb can be used to increase signal-to-noise at the expense of resolution

sb
sine bell; weighting function that uses a sine function; if sb = at, then a pure sine function is applied to data upon wft command; if sb = at and sbs = -at, then a pure cosine function is applied over all of the FID; if sb < 0, then a sine squared function is applied; sb = -at, sbs = -at, then a cosine squared function is used

sbs
shifted sine bell; shifts the function, not used if sb = 'n'

gf
Gaussian function; weighting function that applies Gaussian function; normally broadens line and increases signal-to-noise

gfs
shifted Gaussian function

awc
adjusted weighting constant

Linear Prediction:

proc
type of processing of FID; if proc = ‘lp’ then linear prediction is used; if proc = ‘ft’, no linear prediction is used

backlp
command to automatically setup a backward linear prediction to remove the first few data points of FID

lpopt
linear prediction option- forward lp = ‘f’, backward lp = ‘b’; or both lp =’f’‘, ‘b’

lpfilt
number of linear prediction coefficients, must be greater than the number of signals in the FID, or resonances in the spectrum

lpnupts
number of complex time domain points to be used in the linear prediction, must be > 2*lpfilt, could be set ~np/4 or as great as np/2

strlp
specifies the first complex time domain point to be used in the linear prediction, should be = np/2

lpext
the number of points to extend the FID by, could be set = strlp or as great as = np

strtext
starting point for linear prediction, the point at which the linear prediction begins, should be set to np/2 + 1

Integration/Baseline Correction:

lvl
level for integrals; first mouse click during interactive adjustment of lvl/tlt will only adjust lvl, in essence a zero-order adjustment of flatness of integrals (as with rp for phase correction)

tlt
tilt; second mouse click during interactive adjustment of lvl/tlt will adjust both lvl and tlt, in essence a first-order adjustment of flatness of integrals (as with lp for phase correction)

cz
clear integral reset points

dc
drift correction; a zero-order baseline correction of spectrum, uses lvl/tlt to define what is the baseline

cdc
clear drift correction; removes drift correction

bc
baseline correction; uses integral reset points to define baseline; bc(2) would use a first-order polynomial, bc(3) would use a second order polynomial... bc or bc(1) would use a spline function

dpir
display integral region below spectrum

dpirn
display normalized integral regions; depends upon value of ins

ins
sets integral value of whole spectrum

setint
set integral of a specific peak

dlni
display text of integrals

intmod
integral mode; intmod = ‘partial’ shows partial integrals, = ‘full’ full integral, ‘n’ = no integral

is

integral scale; can be adjusted with middle mouse button in integral mode or by typing is = number or with isadj command

isadj
integral scale adjust; adjusts scale of integrals automatically

io
integral offset; distance in mm from spectrum to integrals

Display parameters:

df
display fid

ds
display spectrum; useful when control over spectral display is lost

wc
width of chart; in mm across screen or page

sc
start of chart; in mm across screen or page

wc2
width of chart in 2nd dimension (vertically in 1D)

sc2
start of chart in 2nd dimension (vertically in 1D)

full
full screen; show spectrum on whole screen

f
full spectrum; display entire spectral width

nl
nearest line; puts cursor on the nearest line

rl
reference line, in Hz by default; if cursor is on the CHCl3 resonance, rl(7.26p) would set the CHCl3 resonance to 7.26 ppm

th
threshold; value of minimum peak in millimeters to be accepted by pll, dll, ppf, dpf commands

sp
start of plot; fix value of minimum ppm value to be shown; for example sp = -0.1p means the start the plot on the screen will be at -0.1 ppm; if no argument is used, for example sp = 0.1, then spectrum will start at 0.1 Hz not ppm

wp
width of plot; fix how many ppm are displayed on screen; for example, wp = 10p will display 10 ppm

dtext
display text as entered with text command

dll
display line list in text form

dpf
display frequencies on resonances

dscale
display scale

vs
vertical scale; can be adjusted with middle mouse button or manually by typing vs = number

vsadj
vertical scale adjust; adjusts vertical scale to biggest peak in displayed spectrum

vp
vertical position; the baseline of spectrum is adjusted on the screen; vp = positive number adjusts vertical position toward top of screen

dps
display pulse sequence on screen

dres
display resolution; displays the line-width at half-maximum intensity for analyzing quality of shims and the digital resolution (the amount of Hz between points)

res
resolution; displays the line-width at half-maximum intensity, 0.55% intensity, and 0.1% intensity; for analyzing shims at both the half-height and the base of the resonance

color
command that opens up a color box where you can use the colors of your spectra, parameters, etc. both displayed and printed

inset
allows for an inset of spectrum to be put on top of spectrum such that one can zoom in on a portion of the spectrum and print that portion on top of full screen

Arrayed Experiments:

array
command to setup a series of values for a parameter; often used in determining the 90° pulse

pad
pre-acquisition delay; the delay at the start of the spectrum before there is any pulsing. The pad is used not between scans, but between members of an array, normally used in kinetics experiments rather than arraying d1, pad is arrayed so that one can acquire at specific times even if nt > 1.

dssh
display stacked spectra horizontally

dssl
display stacked spectra with number on spectra to indicate the arrayed parameter number

dssa
display stacked spectra automatically; display arrayed experiment vertically, rather than horizontally

dss
display stacked spectra; uses wc, sc, ho and vo parameters for space between spectra of array

ai
absolute intensity; scales arrayed experiment so that displayed noise level is same in all values of array

nm
normal mode; scales to largest peak in spectrum (the opposite of ai)

da
display array; displays value of arrayed parameter

ho
horizontal offset; amount of offset of different spectra of array in horizontal direction, used with dss command in combination with a change of wc and sc

vo
vertical offset; amount of offset of different spectra of array in vertical direction

Plotting parameters:

pl
plot spectrum

pap
plot all parameters

ppa
plot a limited set of parameters

pltext
plot text as entered with text command

pll
plot line list in text form

ppf
plot frequencies on resonances

pir
plot integral region

pirn
plot normalized integral regions

plscale
plot scale on spectrum

pps
print pulse sequence

pp
print to paper; switches to HP language output and attached printer, better for printing spectra to paper

pf
print to file; switches to Adobe PostScript output, some attached printers read postscript and will print to paper with page command to attached printer. For instruments without attached PostScript printers, pf will switch printing output to nmr1 printer. To return from PostScript to normal type pp

pcf
print to color file; switches to color output with Adobe PostScript files

page

send plot to printer; if the page command is used with an argument such as page(‘something’) then the plot will be saved to a file; if a postscript printer is selected (by pf or pcf commands) then the file can be transferred to Adobe Photoshop/Illustrator

darkenps
darken postscript plots; makes lines thicker than PostScript default, creates a darker PostScript plot

pstojpg
converts postscript files to jpg files

pstotiff
converts postscript files to tiff files

File Retrieval/Storage and UNIX commands:

svf
save fid; saves fid, parameters, text and log files to something.fid (a directory that will contain fid, parameters (a file called procpar), text, and log files)

svp
saves parameters; saves parameters and text files to something.par

svs
saves shims; saves shim settings to file stored in directory /export/home/username/vnmrsys/shims

rt
retrieve fid; for example rt('something') retrieves something.fid directory

rtp
retrieves parameters; rtp('something') retrieves something.par or parameters contained in something.fid; must type su to load parameters to console

rts
retrieve shims; rts('cdcl3') retrieves shims from file called cdcl3, computer will look first in /export/home/username/vnmrsys/shims directory then in /vnmr/shims directory. Shims can also be retrieved from something.fid. Must type su to load shims after rts command

jexp1
join experiment 1; changes to exp1 parameter set; similarly jexp2 changes to experiment 2 parameter set, etc.

mp
move parameters; mp(1,2) would move parameters stored in exp1 to exp2; mp(2,) would move parameters from exp2 to exp4 ...

mf
move fid; mf(1,2) would move parameters and fid from exp1 to exp2 ...

cd
change directory; UNIX command to change directories; by typing cd without any argument will change to home directory in UNIX terminal or in VNMR window; home directory is /export/home/username; cd('/vnmr/shims') would change to /vnmr/shims directory in VNMR window; cd /vnmr/shims would do the same in terminal window

pwd
present working directory; tells you which directory you are currently working in; should be home directory unless directory was changed

ls
list files in current directory; ls -l would list files in current directory with corresponding sizes

rm
remove file; rm(‘something’) would remove filed called something if typed in VNMR window; rm something would do the same in UNIX terminal; rm -r something.fid would remove directory something.fid (ALL Varian fids are stored in directories)

mv
move file; changes name of file; typing move something.fid some.fid would rename something.fid to some.fid

man
manual; man ls would give the manual entry of ls command in typed in UNIX terminal window; similarly man(‘gCOSY’) typed in VNMR window would give manual entry for gCOSY command

2D Setup Commands:

gCOSY
gradient COrrelation SpectroscopY; gCOSY macro converts 1H 1D parameter set to a gCOSY experiment

TOCSY
TOtal Correlation SpectroscopY; TOCSY macro converts 1H 1D parameter set to TOCSY experiment

gHSQC
gradient Heteronuclear Single Quantum Coherence; gHSQC macro converts 1H 1D parameter set to a 1H/13C gHSQC

gHMBC
gradient Heteronuclear Multiple Bond Coherence; gHMBC macro converts 1H 1D parameter set to a 1H/13C gHMBC

gHMQC
gradient Heteronuclear Multiple Quantum Coherence; gHMQC macro converts 1H 1D parameter set to a 1H/13C gHMQC

ROESY
Rotating Overhauser Effect SpectroscopY; ROESY macro converts 1H 1D parameter set to a ROESY experiment

NOESY
Nuclear Overhauser Effect SpectroscopY; NOESY macro converts 1H 1D parameter set to a NOESY experiment

2D Acquisition Parameters:

nt
number of transients (also referred to as number of scans or acquisitions); often must be a multiple of a specific number (gHSQC, gCOSY, gHMBC, gHMQC must be a multiple of 2; TOCSY must be a multiple of 4, preferably 8; NOESY and ROESY must be a multiple of 8, preferably 16)

bs
block size; amount of scans after which data is written to hard drive; does not have much effect on 2D experiment, could be set = 'n'

sw1
spectral width in t1 dimension (indirectly detected dimension)

p1
pulse width one; sometimes used as second pulse (normally a 1H pulse);

p1lvl
power level of pulse one

slpw
spin lock pulse width; used in ROESY and TOCSY experiment; lower power pulse (must be a 90 pulse at a specific lower power level), must be short enough to excite entire spectral region, but not so short that the required power is too high to cause sample heating, used during spin-lock period (mixing time) of ROESY and TOCSY

slpwr
spin lock power level; used with slpw in ROESY and TOCSY; the power level for slpw pulse

gain
receive gain; the amplification of the signal; higher gain means more amplification

ni
number of increments; amount of t1 points; essentially equivalent to np in t1 dimension, but most likely ni < < np

pwC
pulse width Carbon; 90° pulse at a given power level (pwClvl); used in gChsqc experiment

pwx
pulse width X nucleus; 90° pulse at a given power level (pwxlvl); used in gHSQC, gHMQC, gHMBC experiments

pwxlvl
power level for X nucleus 90° pulse

pwClvl
power level for ^{13}C nucleus 90° pulse

jxh
X-H coupling constant parameter; used to set delay for magnetization transfer between X nucleus and proton

j1xh
1-bond X-H coupling constant parameter; used to set delay for magnetization transfer between X nucleus and proton (used as a 1-bond filter in gHMBC)

jnxh
multiple bond X-H coupling constant parameter; used to set delay for magnetization transfer between X nucleus and proton

JCH
1-bond C-H coupling constant parameter; used to set delay for magnetization transfer between X nucleus and proton

mix
mixing time; time for NOE transfer in ROESY or NOESY, or total spin correlation in TOCSY

phase
parameter to set type of data acquisition; phase = 1 is a magnitude spectrum normally used with gCOSY; phase = 1,2 is a States-Haberkorn detection (quadrature detection), used for everything else

gt1
gradient time 1; length of gradient 1 (not normally set by user)

gzlvl1
gradient power level of gradient 1 (not normally set by user)

2D Processing and Display Parameters:

Processing:

wft2da
weighted Fourier transform two dimensions arrayed (phase parameter); command to process the full 2D for phase sensitive spectra (almost all 2D spectra are phase sensitive except HMBC and COSY). Phase sensitive spectra are those with the phase parameter set = 1,2

wft2d
weighted Fourier transform two dimensions; command to process magnitude spectra such as HMBC and COSY (or gHMBC and gCOSY). Magnitude spectra are those with the phase parameter set = 1.

wft(1)
weighted Fourier transform 1st FID processes the first fid for the purpose of setting phasing and weighting.

wft1da
weighted Fourier transform one dimension; processes the t2 dimension without processing the t1 dimension; useful for setting processing parameters in t1 dimension

fn
zero fill in t2 (the total amount of points that will be Fourier transformed). fn should be set to equal or twice np parameter. fn = np or fn = 2*np. fn = 2*np will give slight improvement in resolution over fn = np; fn = 4*np will give very slight improvement in resolution over fn = 2*np

fn1
zero fill in t1. fn1 should be set to at least twice ni, four times ni will improve resolution a little more. If you want to have a square 2D matrix, fn = fn1. Note that processing will take a lot longer if fn and fn1 are large (2048 or more).

Weighting Functions:

sb
sine bell in t2

sb1
sine bell in t1

sbs
shifted sine bell in t2

sbs1
shifted sine bell in t1

em
exponential multiply in t2

em1
exponential multiply in t1

lb
line broadening in t2

lb1
line broadening in t1

gf
gaussian function

gf1
gaussian function in t1

For phase sensitive experiments (all except COSY and HMBC), a good way to set weighting is:

sb = -at sbs = sb
for F2

sb1 = -ni/sw1 sbs1 = sb1
for F1 (note that ni is the amount of acquired points in the t1 dimension so if you set ni = 128 but abort the experiment after 64 increments sb1 should be set to 64/sw1 not 128/sw1).

scqosine
macro to set sb = -at sbs = sb sb1 = -ni/sw1 sbs1 = sb1
for a cosine squared function

cosine
macro to set sb = at sbs = -sb sb1 = ni/sw1 sbs1 = -sb1
for a pure cosine function

For COSY and HMBC set:
sb = -at/2 sb1 = -ni/(sw1*2) sbs = sbs1 = 'n'

sqsinebell
macro that sets sb = -at/2 sb1 = -ni/(sw1*2) sbs = sbs1 = 'n'
for a sinequared function

sinebell
sb = at/2 sb1 = ni/(sw1*2) sbs = sbs1 = 'n'
for a sine function

cosineroesy
macro to create cosine squared function with a little Gaussian function to lessen truncation wiggles that are a significant problem in ROESY and NOESY

Phase Corrections:

rp
right phase correct in t2

lp
left phase correct in t2

rp1
right phase correct in t1

lp1
left phase correct in t1

Solvent Suppression:

ssfilter
solvent suppression filter; the number is a value in Hz to suppress.

Baseline Correction:

dc
drift correct

bc
baseline correct

dc2d('f2')
does drift correct of F2 dimension in 2D based upon values of level and tilt

bc('f2',0)
does baseline correction in F2 of 2D based upon integral resets points

Linear Prediction:

proc1
sets whether there is or is not linear prediction in 2D (proc1='lp' for linear prediction in t1 dimension; proc1='ft' for no linear prediction in t2 dimension)

setLP1
macro that automatically sets linear prediction parameters for t1 dimension

Display:

vs2d
vertical scale in 2D plot or the noise level of the plot; the middle mouse button will change vs2d

f
full spectrum

full
full screen

sp
start of plot in t2

sp1
start of plot in t1

wp
width of plot in t2

wp1
width of plot in t1

dconi
display contours intensity; with no argument, displays intensity plot (fast to draw, looks poor); can take arguments such as: dconi('dpcon', positive or negative, number of contours, level multiplier/spacing between contours)

dconi('dpcon',10,1.2)
will give 10 contours positive and negative with a spacing factor of 1.2

dconi('dpcon','pos',10,1.2)
for 10 positive contours with a spacing factor of 1.2

dconi('dpcon','neg',10,1.2)
for 10 negative contours with a spacing factor of 1.2

dconi
dcon interactive

dpcon
display plotted contours

dp10
executes dconi('dpcon','pos',10,1.2)

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dpn10
dconi('dpcon',10,1.2)

dn10
dconi('dpcon','neg',10,1.2)
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Printing:

pcon
print contours; takes arguments like dconi, such as:

pcon('pos',10,1.2) page
will print 10 positive contours

p10
executes pcon('pos',10,1.2) page

p10ps
executes pcon('pos',10,1.2)
then asks for filename to save plot as for exporting postscript

n10
executes pcon('neg',10,1.2) page

n10ps
executes pcon('neg',10,1.2)
then asks for filename to save plot as for exporting postscript

pn10
executes pcon('pos',10,1.2) pcon('neg',10,1.1) page

pn10ps
executes pcon('pos',10,1.2) pcon('neg',10,1.1) page
then asks for filename to save plot as for exporting postscript

plcosy(10,1.2,1)
prints 1H/1H 2D with 10 contours, a spacing factor of 1.2 and a spectrum with 1D on side and top if the 1D is in experiment #1

plcosyps(10,1.2,1)
saves 1H/1H 2D with 10 contours, a spacing factor of 1.2 and a spectrum with 1D on side and top if the 1D is in experiment #1 to a file (the macro will ask for filename)

plhxcor(10,1.2,1,2)
prints 1H/X 2D with 10 contours, a spacing factor of 1.2 and a spectrum with 1D 1H on top if the 1D is in experiment #1, and 1D X on side if the 1D is in experiment #2

plhxcorps(10,1.2,1,2)
saves 1H/X 2D with 10 contours, a spacing factor of 1.2 and a spectrum with 1D 1H on top if the 1D is in experiment #1, and 1D X on side if the 1D is in experiment #2 to a file (the macro will ask for filename)