VNMRJ COMMANDS AND PARAMETERS

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1. INTRODUCTION

All of the buttons used in the VnmrJ GUI to change NMR experimental parameters, start NMR experiments, plot NMR data, etc. have associated letter equivalents that can be inputted into the command line at the top of VnmrJ. The advantage of using the command line over the GUI is simply speed; it is much faster to use the command line. In VnmrJ, there are two main types of input values that can be used in the command line: commands and parameters.

Commands

Commands perform a certain action, such as starting an NMR experiment or printing an NMR spectrum. The syntax is simply to issue the command name into VnmrJ's command line, hit enter, and an action will be performed by the spectrometer. Multiple commands can be used in the same command line and the commands will be performed in the order in which they were inputted into the command line. In these notes, all commands will be in `Courier New` font. Some examples of frequently used commands are:

`time`	displays the total time for the NMR experiment
`au`	starts the NMR experiment, then processes and saves the NMR data when the experiment is complete
`f full aph vsadj`	displays the full spectral width of the NMR spectrum (`f full`), performs an automatic phase adjustment (`aph`) and automatically adjusts the vertical scale of the NMR spectrum so the tallest peak in the spectrum is at the top of the display window (`vsadj`).

Parameters

Parameters are variables that have a specific value assigned to them. The value can be a number or some specific setting. In these notes, parameters will be in Arial font. In VnmrJ, you can see the value of a parameter by typing the parameter name followed by a question mark (eg. nt?) and set a parameter value by typing the parameter name followed by an equal sign and then the value (eg. nt=16). Some parameters have default units that you have no control over, but must be aware of (eg. d1 is in seconds). Unlike when you input a command, when you input a parameter into VnmrJ's command line, no action will be performed by the spectrometer. Parameters are simply utilized by commands and only commands generate a spectrometer response. Similar to commands, multiple parameters can be set on the same input line. In addition, both commands and parameters can be on the same input line. Some examples of commonly used parameters and their usage are:

nt?	displays the current value of the number of scans to be used in the NMR experiment
nt=16	set the number of scans to 16
lb=2 `wft`	sets the line broadening to 2 Hz (lb=2) and processes the 1D NMR data (`wft`)

2. GENERAL COMMANDS

The commands described in this section are not found in any of the VnmrJ panels and can be used before an NMR experiment is started.

Table 2.1. General Commands

Command	Example	Stands For	Description
`jexp#`	`jexp2`	join experiment	switches to a different experiment where the experiment number follows jexp; eg. `jexp2` switches to experiment 2
`unlock(#)`	`unlock(2)`	unlock experiment	unlocks a locked experiment; used after the jexp command if the experiment you are changing to is locked
`qtune`	`qtune`	qtune	enters the qtune program used to tune a probe
`su`	`su`	setup hardware	sets up spectrometer hardware and implements changes; must be used before tuning the probe

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3. START COMMANDS

The commands described in this section all have associated buttons that can be found under the Start tab.

Table 3.1. Start Commands

Command	Stands For	Description
`e`	eject	initiates high-pressure air used to eject the sample
`i`	insert	dissipates high pressure air and inserts the sample; always use `e` first, then `i`

4. ACQUISITION PARAMETERS AND COMMANDS

The commands and parameters described in this section all have associated buttons that can be found under the Acquire tab. Among other things, they determine the experimental parameters, plus start and stop the experiment.

Table 4.1. Acquisition Parameters

The parameters change how the actual experiment is performed and are to be set before starting the experiment.

Parameter	Syntax	Stands For	Description
bs	bs? bs=#	block size	after a specified number of scans (the block size), the data will save to a temporary file and can be processed and displayed
ct	ct?	completed transients/scans	displays the number of scans that have completed
d1	d1?, d1=#	relaxation delay	sets the delay used between scans; units of seconds
ni	ni? ni=#	number of increments	specifies the number of increments used in a 2D experiment; generally 64, 128 or 256
nt	nt? nt=#	number of transients/scans	sets the number of scans in a 1D experiment or the number of scans per increment in a 2D experiment

Table 4.2. Acquisition Commands

These commands change some acquisition settings, plus start and stop an NMR experiment.

Command	Stands For	Description
`aa`	abort acquisition	stops the experiment immediately and reports an error; does not process or save data
`halt`	halt acquisition	stops the experiment immediately, processes and saves data
`au`	auto acquisition	begins the experiment and the spectrum automatically processes and saves when complete
`ga`	get acquisition	begins the experiment and the spectrum automatically processes when complete; does not automatically save data
`movetof`	move transmitter offset	sets the centre of the NMR spectrum to wherever the single cursor is positioned; to use, first place the cursor wherever you would like the centre of the spectrum to be, then enter `movetof`
`minsw`	minimize sweep width	changes spectral region to the region selected by the double cursors; must first acquire a spectrum, use the double cursors to select a desired region, then apply `minsw`
`time`	display experiment time	displays the approximate time required to complete the NMR experiment.

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5. PROCESSING PARAMETERS AND COMMANDS

The commands and parameters described in this section all have associated buttons that can be found under the Process tab. They are used to process the data, analyze the data and print spectra.

Table 5.1. Processing Parameters

These parameters can affect how the spectrum appears. There are several different functions that can be used, but most commonly we use line broadening in order to increase signal-to-noise.

Parameter	Syntax	Stands For	Description
lb	lb? lb=#	line broadening	sets the line broadening value, which is applied with `wft`; in general lb should be set to some value between 0.5 and 5

Table 5.2. Processing Commands

These commands transform the NMR data into an NMR spectrum and change the appearance of the spectrum.

Command	Stands For	Description
`aph`	automatic phase adjustment	automatically phases the peaks to pure absorption
`aph0`	automatic phase adjustment	alternate method to automatically phase the peaks to pure absorption; use if `aph` doesn't work
`aphx`	automatic phase adjustment	alternate method to automatically phase the peaks to pure absorption; use if `aph` doesn't work
`bc`	baseline correction	applies baseline correction; must integrate desired peaks first
`process`	process	macro that automatically processes 1D or 2D data
`rl(#.#p)`	reference line	sets the cursor to the chemical shift value specified in brackets; to use, place the single cursor on the peak of interest and use `rl(#.#p)` command to set the reference
`savefid`	save FID	saves the FID using the values specified in the Start → Standard page
`wft`	weighted Fourier transform	applies any weighting functions, processes and displays a 1D spectrum
`wft2d`	weighted Fourier transform	transforms both dimensions of a 2D data set

Table 5.3. Display Parameters*

After the spectrum is processed, these parameters affect how the spectrum is displayed.

Parameter	Syntax	Stands For	Description
`sp`	sp? sp=#p	start plot	specifies the right-hand side start value for a 1D spectrum or the F2 dimension of a 2D spectrum in ppm
`sp1`	sp1? sp1=#p	start plot F1 dimension	sets start plot value (top of the F1 dimension) for the F1 dimension in ppm
`vp`	vp? vp=#	vertical position	controls the position of the spectrum baseline in the screen; increasing vp raises the position of baseline of the spectrum
`vs`	vs? vs=#	vertical scale	controls the peak heights in the spectrum; increasing vs increases the peak heights
`wp`	wp? wp=#p	width plot	sets the width of the plot of a 1D spectrum or F2 dimension of a 2D spectrum; the left-most part of the spectrum will be the sum of sp+wp
`wp1`	wp1? wp1=#p	width plot of F1 dimension	sets the width of the plot of the F1 dimension of a 2D spectrum; the bottom part of the spectrum will be the sum of sp1+wp1

*To see the effect of these parameters, you will need to issue a `ds` (for 1D) or a `dconi` (for 2D) after the parameter is set.

Table 5.4. Display Commands
After the spectrum is processed, these commands affect how the spectrum is displayed.

Command	Stands For	Description
`centersw`	centre sweep width	snaps the cursor to the centre of the spectrum
`dcon`	display colour map	displays a colour plot of a 2D spectrum
`dconi`	display contour plot	displays a contour plot of 2D spectrum
`df`	display FID	displays the FID of a 1D spectrum or FID or the first slice of a 2D spectrum
`ds`	display spectrum	displays a 1D NMR spectrum
`f full`	full spectrum	displays the full spectral width of the 1D spectrum
`nl`	nearest line	snaps the cursor to the nearest peak; often used before `rl` or `movetof`
`vsadj`	vertical scale adjustment	automatically adjusts the peak heights to fill the screen

Table 5.5. Analysis Parameters
These parameters are used when determining the chemicals shifts and integrals.

Parameter	Usage	Stands For	Description
io	io? io=#	integral offset	when integrals are displayed, moves the integral lines up or down; when set to 0, bottom of integral is flush with spectrum baseline
is	is?, is=#	integral scale	when integrals are displayed, controls the height of the integral lines
lvl	lvl=?, lvl=#	level	when integrals are displayed, controls the level of the integrals
tlt	tlt=?, tlt=#	tilt	when integrals are displayed, controls the tilt of the integrals
th	th?, th=#	threshold	determines the minimum peak height required for peak picking

Table 5.6. Analysis Commands
These commands are used when analyzing the processed NMR spectrum, specifically the chemicals shifts and integrals.

Command	Stands For	Description
`dpf`	display peak frequencies	displays the chemical shifts of the peaks above the threshold value
`dpir`	display integral returns	displays the integral values below the peaks

Table 5.7. Printing Commands
These commands are used to determine what should be printed and send the desired items to the printer.

Command	Stands For	Description
`page`	send plot to the printer	sends the plot to the printer; usually preceded by `pl pscale ppa pir ppf`
`pap`	print full acquisition parameters	plots all acquisition and processing parameters; must be followed by `page` to actually print the spectrum
`ppa`	print basic acquisition parameters	plots only the most important acquisition and processing parameters; must be followed by `page` to actually print the spectrum
`pl`	print spectrum	plots the spectrum; must be followed by `page` to actually print the spectrum
`pltext`	print text	plots the text entered in the Comments section in the Start → Standard page; must be followed by `page` to actually print the spectrum
`pir`	print integral returns	plots the integral values below the peaks; must be followed by `page` to actually print the spectrum
`ppf`	print peak frequencies	plots the chemical shifts above the peaks; must be followed by `page` to actually print the spectrum
`pscale`	print spectrum scale	plots the spectrum scale; must be followed by `page` to actually print the spectrum
`plot`	print macro	general plotting macro that plots 1D and 2D spectra; automatically prints spectrum with scale, acquisition parameters, peak picks and integrals (for 1D), F1 and F2 projections (for 2D)