Using VnmrJ for Spectral Processing

Opening VnmrJ

You will need X11 software downloaded. The following links should help:

Windows: http://sourceforge.net/projects/xming/
Mac: http://xquartz.macosforge.org/landing/

In addition, if you are not connected to the UCSF WiFi (UCSFwpa), you will need the following Junos Pulse (VPN) software:

http://software.ucsf.edu/applications/vpn.html

When you run the software, type https://remote.ucsf.edu/pulse in the "Sign in at:" field. You will need your UCSF MyAccess ID (SF######) and password to login.

The VNMRJ program is on the 'grase' workstation on the radiology network. The following user accounts are available for users:

- user1
- user2
- user3
- user4
- test

If you have problems trying to login remotely, try logging in directly to the user account using the radical workstation in room BH-102.

Open a terminal from a Linux workstation on the radiology network or from a Mac connected to the UCSFwpa or VPN:

- ssh –X user2@grase.radiology.ucsf.edu
  enter password: 1varian1
- vnmrj -this will start the vnmrj program

If you are using the radical workstation, login to the user account and click on the VnmrJ icon.

1. Using the File menu or rt command, load the file

You can also install VnmrJ on a Mac only (requires Java to run)

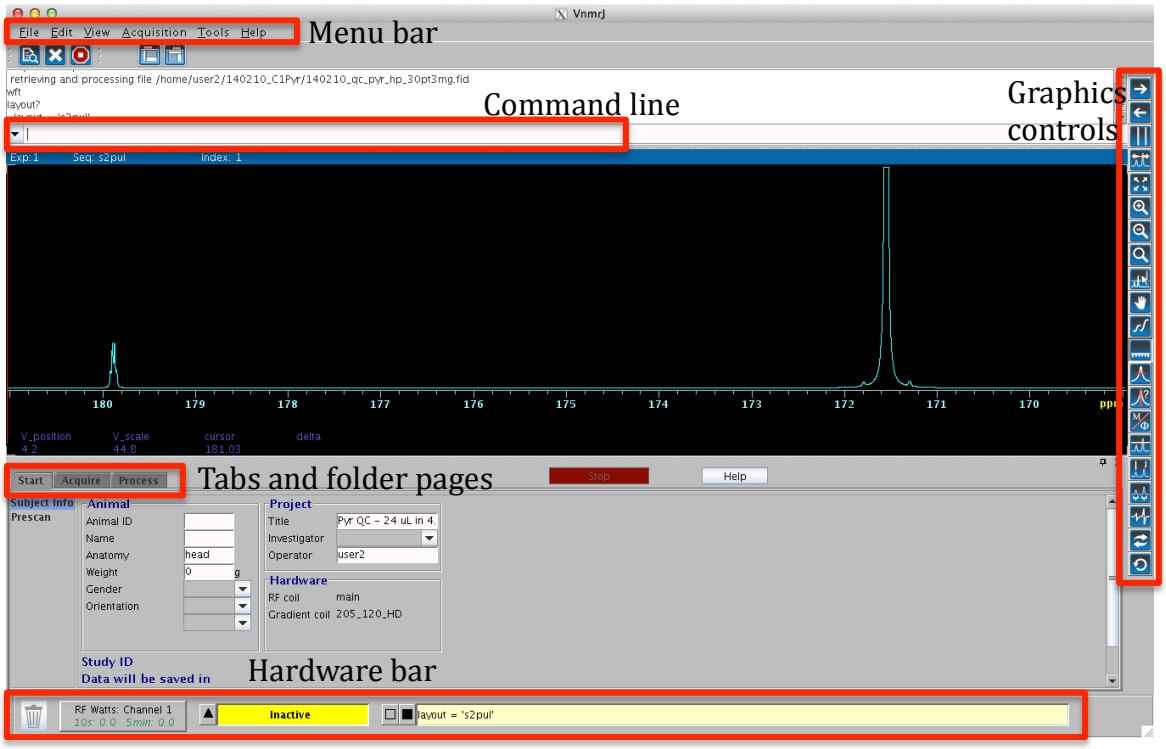
*NOTE: If VnmrJ starts with "Exp: 0" displayed in the upper lefthand corner (see below), type the following:

- jexp# - changes experiments (# is any number, eg. 2, 3, 4, etc.)

To load FID

a) Select “Review” Viewport → load file using File Browser.
    a. Data is located in /home/vnmr1/class_demo/test_data_2016/
    b. 13C spectra: 13C_1_C1C2Pur_copol_LnCaP_021716.fid
    c. 31P spectra: 31P_1_LnCaP_021716.fid

VNMRJ - Graphical User Interface



Display FID
Display spectrum

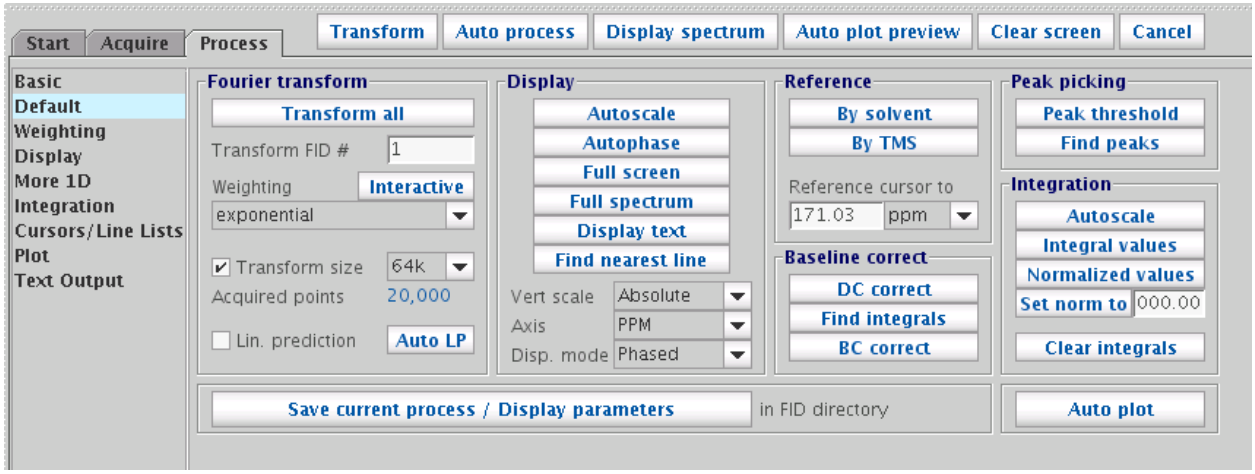
Increment (next spectrum)
Decrement (previous spectrum)
Toggle between 1 cursor, 2 cursors
Show full spectrum
Reset to full display
Zoom in
Zoom out
Zoom mode
Interactive array spectra
Pan & stretch mode
Show integral regions
Show/hide axis
Measure linewidth
Frequency at cursor
Magnitude/phase mode
Show/hide threshold
Pick and display peaks above threshold
Display integral values
Phase mode
Redraw
Return

Show integral regions

Show full integral
Define integral regions
Integral level/tilt

Process data

The Process tab contains the GUI for processing NMR data.



a) Fourier transform by clicking 'Transform' or by typing the command:
   - wft - apodize (digital filter) and FT

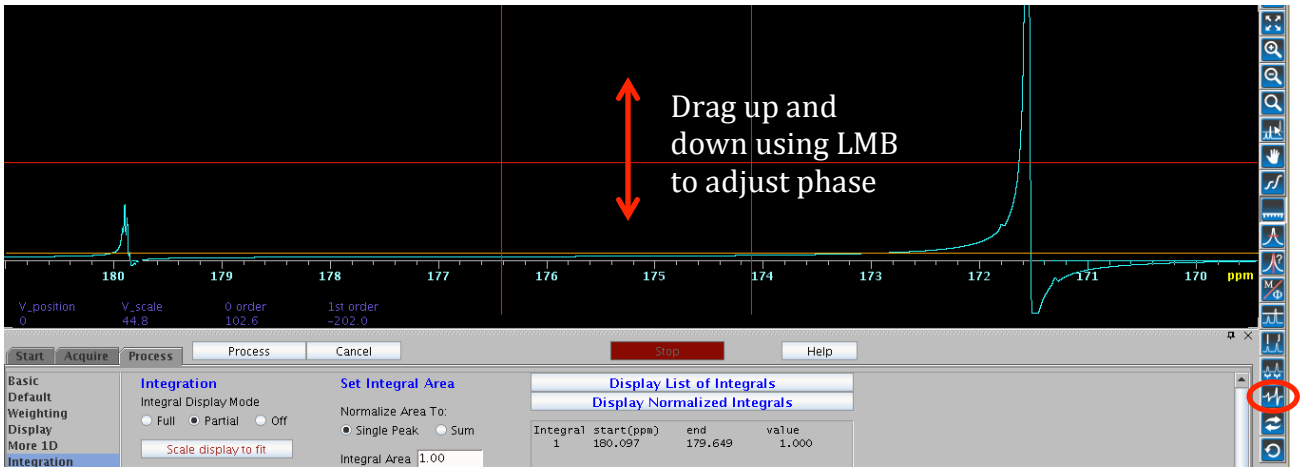
b) Select and display region of interest
   a) Use the LMB and RMB to position the left and right line cursors on the spectrum
   b) Click on the 'magnifying glass' icon to zoom

c) Adjust height of peaks using the middle scroll button, or by typing the command:
   - vsadj - adjusts vertical scale for tallest peak in spectrum

<u>Phase correction</u>

(A) Autophase
   - aph0 – apply zero order correction
     OR
   - aph - apply 1st and zero order phase correction

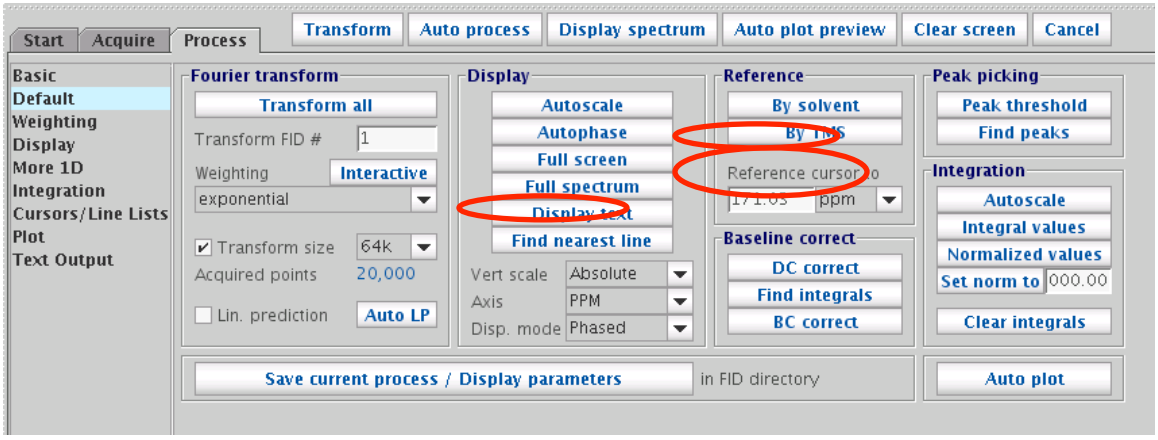
(B) To manually phase correct the spectrum:
   i) Click on the 'Phase' icon
   ii) Move the cursor on a peak towards the right of the spectrum
   iii) Press the LMB and move the cursor vertically to adjust the phase of the peak to make it upright
   iv) Move the cursor to a peak towards the left
   v) Press the LMB and adjust the phase of the peak
   vi) Repeat (iii) to (v)



Referencing a peak to a particular ppm value

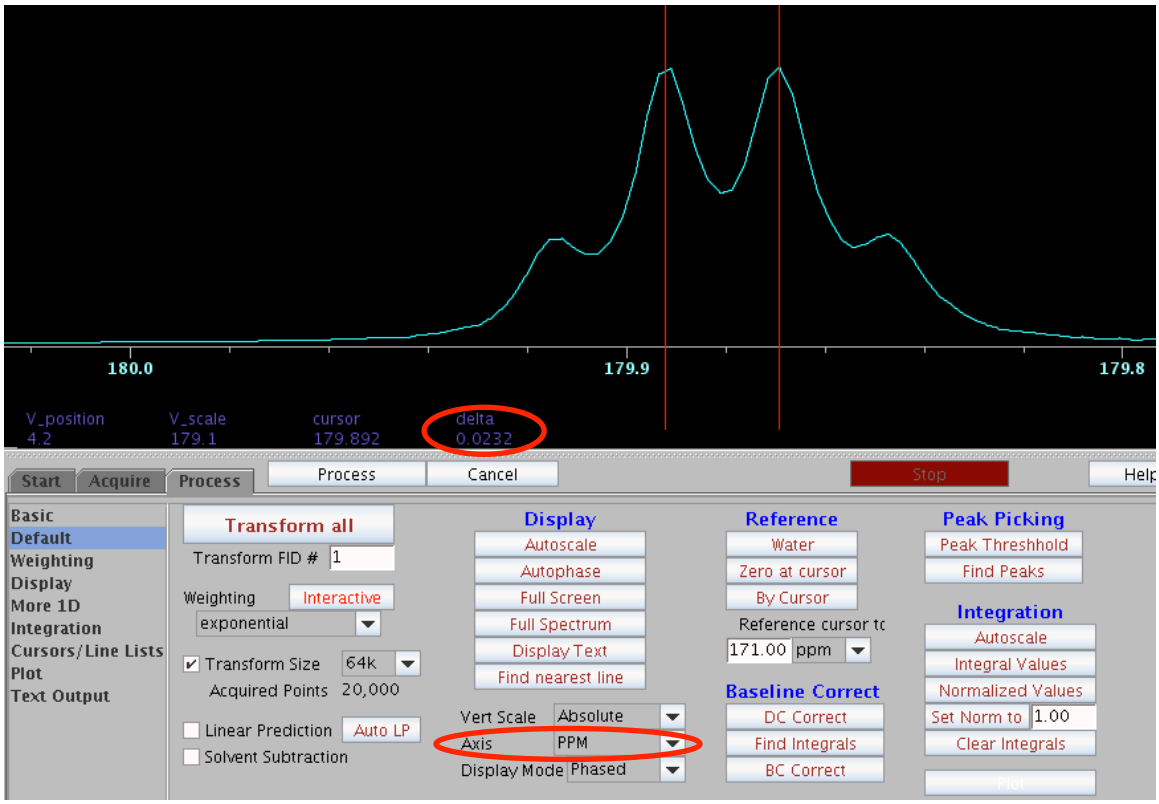
a) Select the peak - Set the (left) cursor on the peak
- nl -set cursor on the nearest line

b) Enter the chemical shift of the reference peak
- rl(4.5p) -reference line, ppm



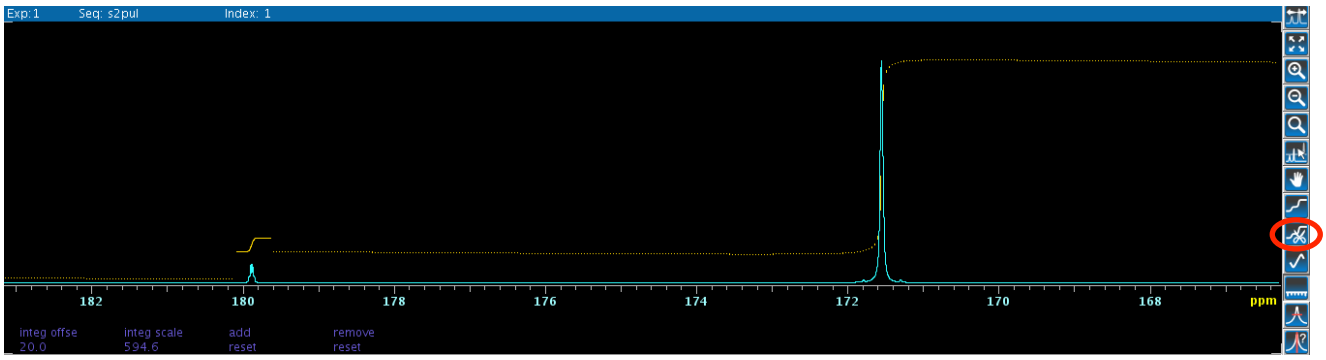
Measuring chemical shift differences

a) Under the Default tab, set the Axis to the desired scale (typically Hz or ppm; see image below)
b) Use the LMB to set the left cursor on the downfield peak of interest
c) Use the RMB to set the right cursor on the upfield peak of interest
    a. The chemical shift difference is displayed below the spectrum (see image below)

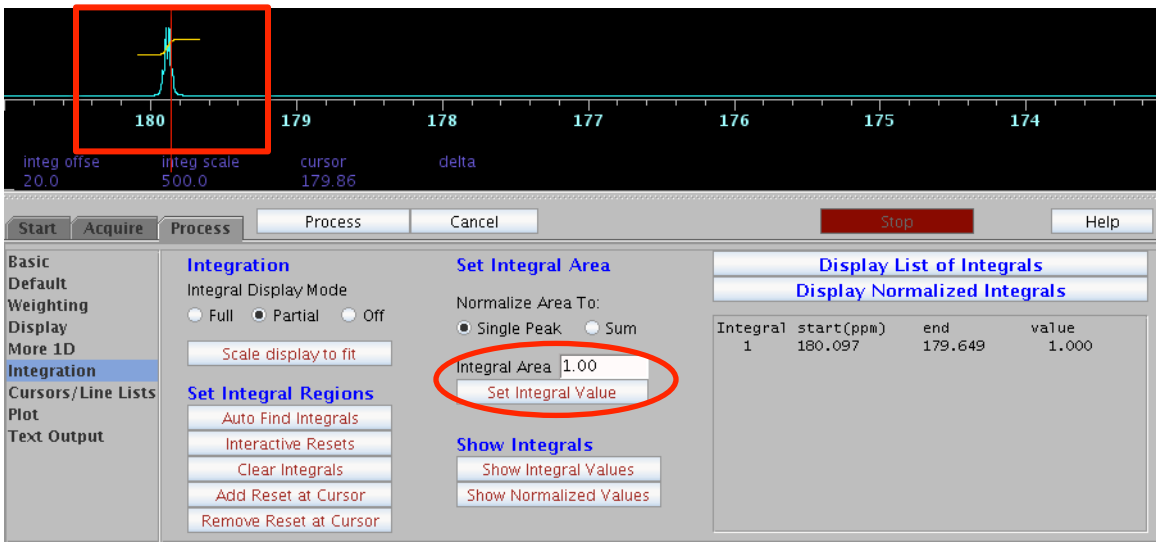


Quantifying peak integrals

a) Click on the Show integral regions button on the sidebar
    a. New buttons appear (see below)
b) Adjust vertical scale of integrals using middle scroll button
c) Click on the Define integral regions button, click to the left and to the right of the peak to define the integral region

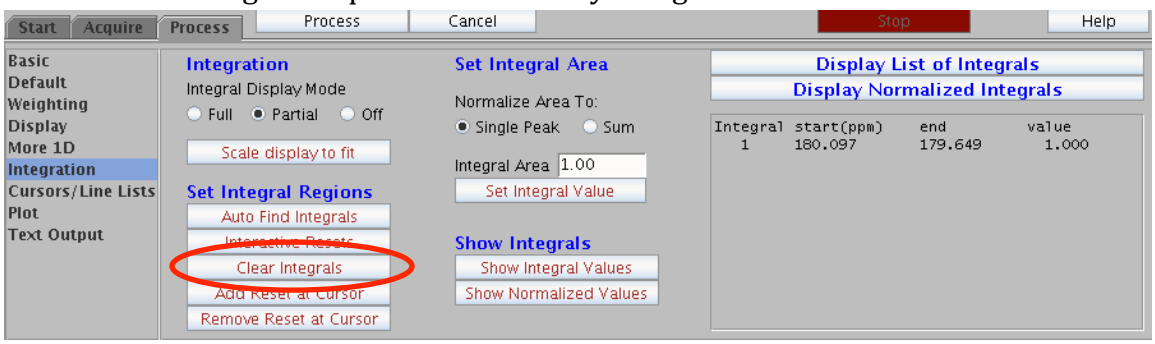


d) To set integral value:
    a. Place red cursor anywhere on integral area of interest
    b. In the Integration pane, set Integral Area as desired, click Set Integral Value button



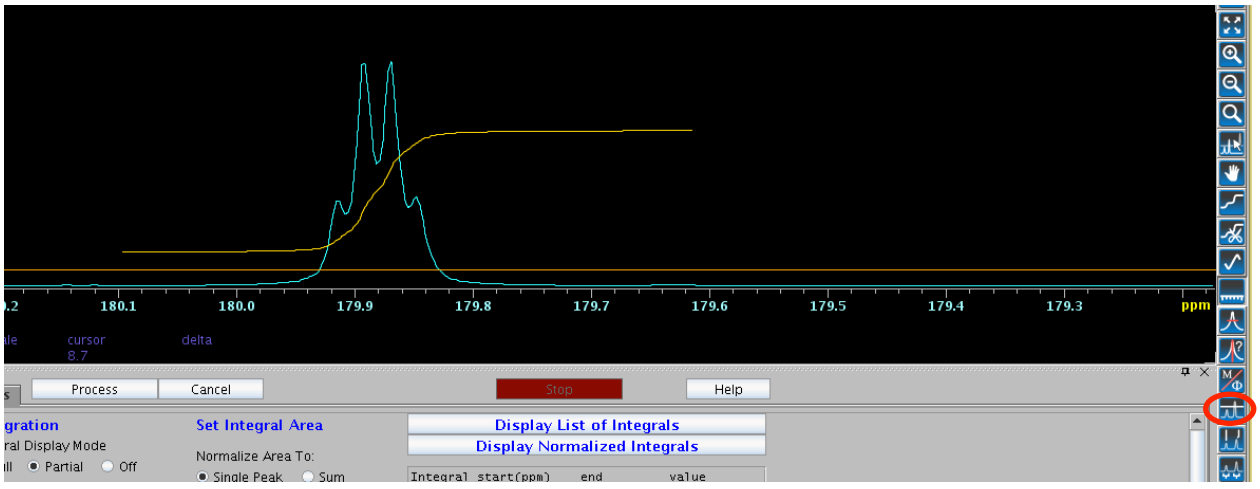
<u>T_1 fitting</u>

a) *Clear all previously defined integral regions* by clicking on the Clear Integrals button in the Integration pane – otherwise you'll get an error!



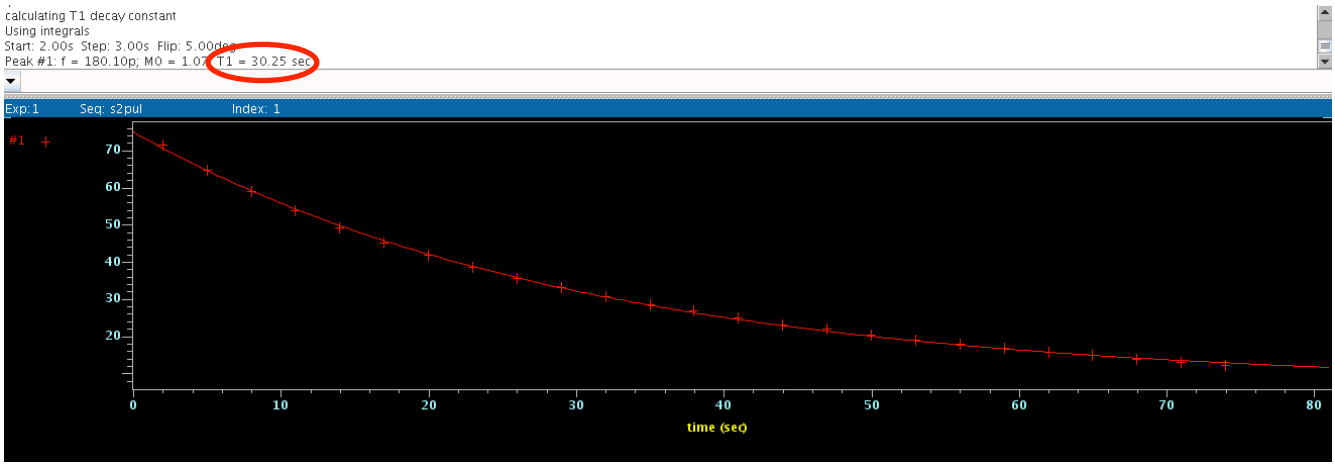
b) Define the integral region of the peak of interest, as explained above

c) Click on the Set threshold button on the sidebar, and set it so it is just above the base of the peak



➢ hpt1 - initializes the hpt1 macro for T_1 fitting

- Enter the magnet-to-polarizer transfer time when prompted (doesn't affect the calculated T_1)
- Enter the TR (in seconds) when prompted
- Enter the flip angle (in degrees) when prompted



Exiting VnmrJ

Please be sure to exit VnmrJ before logging out! This can be done by:

1. Closing the window
2. Typing "exit" into the command line

References:

VNMRJ Help files on the web
There are a number of help files on the web for acquiring NMR spectra on a Varian scanner. A few selected references are listed here.
Please note that the VNMRJ software installed on the 500-Inova is the version 1.1D. The current version is 4.0. The software can also be installed on Linux or Windows based PC's and on Apple computers.

Using ***VnmrJ*** to process simple NMR spectra - YouTube
www.youtube.com/watch?v=1zd0krRrVY4
-Youtube video; For processing only

Using **VNMRJ** - 1D Proton NMR - **YouTube**
www.**youtube**.com/watch?v=mmn5k9Doo-U

-Youtube video; routine acquisition and saving of proton spectra; newer vnmrj version

PROCESSING 1D SPECTRA USING **VNMRJ**
http://publish.uwo.ca/~chemnmr/usingthefacility/Processing_1D_VNMRJ32_1.0.pdf

VNMRJ User's ***Guide*** (pdf)
http://chem-faculty.lsu.edu/nmr/VnmrJ_Intro011808.pdf

Vnmrj Training ***Guide*** - University of Michigan
www.umich.edu/~chemnmr/docs/UM_NMR_Training_2011.pdf

VNMRJ-intro - Biomolecular NMR facility
utswbionmr.swmed.edu/UserMan_Site/web-content/Index.html
-gradient shimming included; figures showing cable connections

VNMRJ on Mercury400 NMR Operating ***Instructions***
www.emory.edu/NMR/.../VNMRJ%20%20Operating%20Instructions.pdf
-command descriptions included

Guide to Varian Spectrometers running ***VnmrJ*** - Biomolecular **...**
http://www.ucdenver.edu/academics/colleges/medicalschool/programs/biomol/strucbiocores/nmr/Documents/pdf/UCDHSC-VNMRJ-NMR-GUIDEv3.pdf
-well organized manual; 1H and 2H gradient shimming included; lot of details

How-to Sheets for popular NMR experiments and procedures.

www.chem.uky.edu/Resources/NMRexperiments_Fall2010.html
-brief and detailed instructions for a lot of experiments; vnmrj2.2;

VnmrJ Manual
www.chem.csi.cuny.edu/**VnmrJ**.pdf
-brief instructions, 4 pages; vnmrj1.1d
Chemistry Department
www.k-state.edu/chem/downloads/1dvnmrj.pdf
-basic instructions for acquiring 1H and 13C spectra; vnmrj1.1

WORKING UP 1D NMR SPECTRA USING ***VNMRJ*** **...** - Publish Uwo
publish.uwo.ca/~chemnmr/.../Processing_1D_VNMRJ32_1.0.pdf
-processing only; vnmrj3.0;

VNMRJ 4.2 – Manual
http://pcweb.ucsf.edu/UCSF-NMR/pdfs/VnmrJ4_manuals/SpecUsers_G7446-90573.pdf

Updated: 2/26/15
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