

## **NMR Instructions—Offline in the Schupflab** **To log on/load your file**

1. Log onto the computer (Linux OS) by using Login = chem  
Password = keyes404
2. Double-click the “walkup data” folder on the desktop
3. If you are asked for a password, enter “keyes208”
3. Drag the folder containing your spectrum onto the desktop (see *Directory 1* in Fig. 1)
4. Close the “walkup data” folder
5. Double-click the VNMRJ icon to open the NMR program
6. Go to File → Open (pull-down menu, top-right of window)
7. Find your file and double-click on it to open; to do this in general you will have to:
  - (1). Make sure the File Type pull down menu is set to “All Files”
  - (2). Go up 2 or 3 levels to the “desktop” folder
  - (3). Double-click the desktop folder
  - (4). Double click on your data folder on the desktop (*Directory 1* in Figure 1)
  - (5). Double click on the folder with the Sample ID as the file name (*Directory 2*)
  - (6). Double-click the “data” folder
  - (7). Double-click your file with extension “.fid” (*Directory 3*)

***When you are finished at the end of the session, please drag your desktop folder to the trash, and empty the trash!***

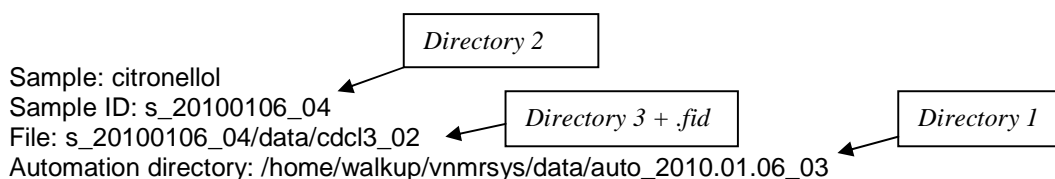






Figure 1: Typical file header (upper left-hand corner of your spectrum plot).

### ***Manipulate Your Spectrum***

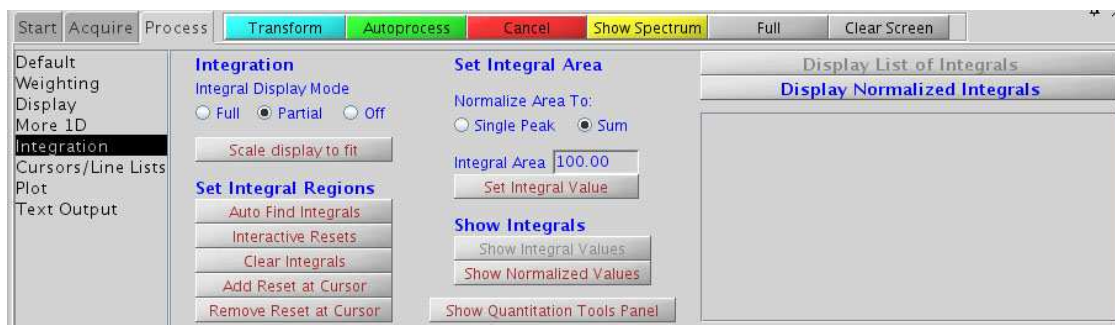
The graphics bar (right of this page) will appear at the upper right side of the screen. You will need to use these buttons and the mouse/cursor to manipulate your spectrum. [If the cursor bar does not appear, pull down the View menu, slide right on the Tools entry and choose the graphics bar.]



***Expand/zoom on the x-axis*** – use the left and right mouse buttons to define a region on your spectrum between the two red vertical lines (you may need to press the  button first). Press the (+)-magnifying glass button  to zoom to the defined region. Press the (-)-magnifying glass button  to zoom back out, or the  button to view the entire spectrum.



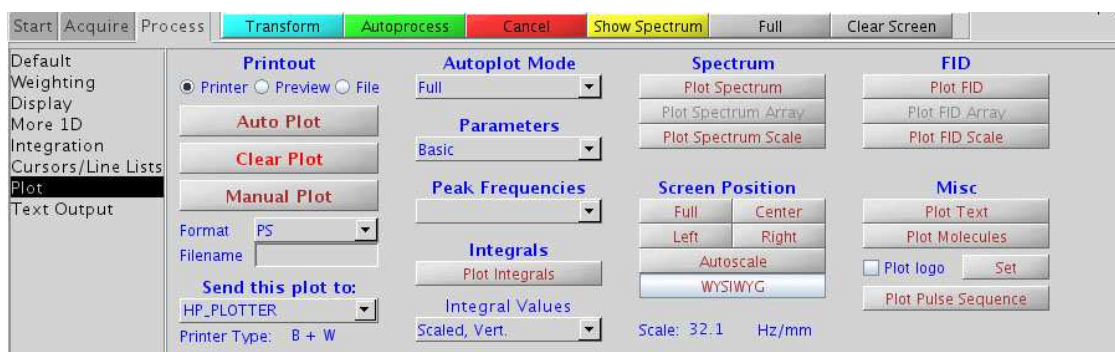
**Expand/zoom on the y-axis** – place the cursor over a peak that you wish to expand, and then press the middle mouse button – your spectrum will expand the peak vertically to match the position of the cursor.

## Integration



In the lower-right window, press the “process” tab and then select integration from the menu. First press the integration button  until the integral line is visible on the spectrum (you may have to press it twice). Then press “clear all integrals” followed by “interactive resets”. Define your integral regions (where you want it to integrate) by pressing the left mouse button on either side of the region that you wish to integrate. Repeat for each integral region. When you are done, press the integration button  to turn the integrals off (the integrals should no longer be visible).

## Printing your spectrum



Make sure that the region you wish to plot is displayed on the screen. In the lower-right window, press the “process” tab and then select the “plot” page. Change the Autoplot Mode to “As Displayed” and then click the Auto Plot button. Alternatively you can specify what is plotted. For example, press the following five buttons (in order): “plot spectrum”; “plot spectrum scale”; “plot text”; “plot integrals”; then the “Manual Plot” button.

**When finished pull down the File menu in VNMRJ and choose *Exit VNMRJ***