^{1}H Operating Instructions for the Old Software (2006)

(Currently for INOVA 400, INOVA 600, Mercury 300)

Taking A Proton NMR

1. Record your name, research group, spectra to be taken, and login time in the login book.

2. Load your sample, lock and shim it. (See Locking and Shimming Instructions for old software)

3. Type **h1** to load the standard parameters for a 1D ^{1}H spectrum in $CDCl_3$. If your solvent is not deuterated chloroform, type **h1('***solvent name***')** to load the parameters for that solvent.

4. Type **nt=x** where x = the number of scans you want to take. Normally this number is 8 or 16 (multiples of 8 should be used). Dilute samples may take more scans. Then type **ga** to begin taking scans.

5. Once the acquisition is complete, type **wft** to work the Fourier transform then **vsadj** to adjust the peaks to the screen. You can adjust the spectrum height at any time using **vsadj**.

6. Type **aph** to automatically phase the spectrum. Occasionally the auto phase command does not work well. In these cases you must phase manually by clicking on the **phase** button, then clicking on a peak and using the left and right mouse buttons to phase your spectrum.

7. You next need to set the reference. Press the button called **dscale** to display the scale on screen. People usually use the solvent peak as a reference, but you may use an internal standard if you wish. To see the

reference, place the cursor close to the solvent peak and type **nl** to move the cursor precisely on top of the peak. Next type **rl(**XX.X**p)** in order to set the exact chemical shift of the reference peak. You can find a list of solvent peak values near every NMR.

8. You may expand on a specific region of your spectrum by clicking with the left mouse button to set one cursor, then clicking with your right mouse button to set a second cursor. This will form a box around an area of your choosing, which you can zoom in on by pressing the **expand** button. To return to the full spectrum click on the button called **full**. Alternatively, you can expand on a specific region by typing **cr=**XX.X**p** to set the left cursor value, and then **delta=**XX.X**p** to set the right cursor X ppm away upfield from the left cursor, then press **expand**.

9. To integrate the spectra, first click on the **part integral** button. Then click on the button labeled as **resets**. **Resets** allows you to cut the integral line by pressing the left mouse button. Make cuts on each side of the peaks such that all peaks are present in one integral, then type **bc cz**. The **bc** command will correct the baseline of the integral, and **cz** will erase the cuts you have made. You can also baseline correct the integral manually by clicking on the **Lvl/Tlt** button and then using the left and right mouse buttons to adjust the line, then type **ds** to return to the spectrum. Once the integral line has been leveled, you can cut integrals for each of your peaks by pressing the **resets** button again, and cutting around each peak using the left mouse button. Once you have finished integrating, you should set a standard integral value. Place the cursor over a peak you wish to assign, then press the **Set Int** button. You will be asked to assign an integral value, type in the number you wish to set the peak to. To display the integrals on screen, type **dpir**.

10. You may label your spectrum by typing **text(‘***spectrum name***’)**.

11. To print, first type **vp=12** to adjust the spectrum to a vertical height the printer will recognize. There are then a variety of printing commands. Use any commands you wish, but they should be entered in a single line, with **page** as the last command.

Example: **pl pap pir pscale page**
(this will print the spectrum, the parameters, the integrals and the scale)

a. **pl** – prints the spectrum
b. **pap** – prints acquisition parameters
c. **pir** – prints integrals
d. **ppa** – prints an abbreviated acquisition parameters list
e. **pltext** – prints text label
f. **pll** – prints peak frequencies as a list
g. **ppf** – prints peak frequencies above each peak
h. **pscale** – prints the scale
i. **page** – sends print commands to the printer

12. It is recommended that you save most spectrum. You must first create a directory, you can do this by typing **mkdir(‘***directory name***’)**. If the directory you want to save in already exists, you may access it by typing **cd(‘***directory name***’)**. To save the spectrum type **svf(‘***spectrum name***’)**.

13. In order to retrieve a saved spectrum, you must first access the directory you saved it to in the same way as above. Click the **file** button, highlight the spectrum you want to view, and click **load**. Then type **wft** and your spectrum will appear on the screen.

14. When you are finished, re-insert the standard $CDCl_3$ sample, lock it and shim it (see Locking and Shimming instructions for old software). Then type **h1**, then type **exit**. Then right click on the desktop and select **logout**. Make sure you completely logout.

15. Make sure to record your logout time in the logbook.