Operation Procedure for Varian 500 NMR

1. Login with you username
2. Password
3. Click on “VNMRJ” on the desktop
4. Click on “eject” or type “e” in the command line to eject sample
5. Click on “inject” or type “i” in the command line to insert sample
6. Click on “new study”
7. Select experiment by clicking on “PROTON” or “CARBON” or whatever other experiments you want to set up in the top left panel
8. Type in sample name and comments
9. Uncheck “autoplot” if you don’t need it, because you will process data and take the printout by yourself
10. The default scan number is 8, but you can change the scan numbers by double clicking on the proton icon (the one you just selected) on the lower left column, then go to “defaultH1”, select desired scan numbers and spectral width to whatever you want it to be
11. Submit
12. Type “wft” or “ds” to display spectrum
13. Process data (similar to the old software)

    13-1. Type “cz” to clear all integration done by system or the previous integration you have done

    13-2. Type “vp=12”. This is to plot calculated integral values below the spectrum, the spectrum must be at or above a vertical position of 12.

    13-3. When you select **“Integration”** in the **“process”** submenu, you can do the following:

    ---**Integration**-click on the “Set integral region” button on the right side of the spectrum window (you can see the function of each icon when you place your cursor on that icon for 2 seconds), then you will see an icon with a scissor in the center which is “Define integral region”, click on it and you can do the integration simply by left clicking the mouse on both side of a peak as what you did before.

    ---**Set integration value**: put cursor on a peak that you want to set as a specific value, select “single peak”; in the “integral area”, type in a value in the box below, for example “1” or “2, then click on “set integral value”.

    ---**Adjust vertical height of the spectrum**, in the “integral”, you have three options: “full”, “partial”, “off”, select **“off’**, and middle click on the roller of the mouse and hold it, drag it up and down to adjust the height of the spectrum. But when you want to do the integration, you have to do it in either “full” or “partial” mode.

13-4. When you select **"Display"** in the **"process"** submenu, you can do the following:

---Reference a peak to a specific chemical shift, for example set up the CDCl3 peak as 7.27. Put the cursor on the peak that you want to reference to, go to "reference cursor to___ppm", type in the value in the blank area.

13-3. When you select **"plot"** in the **"process"** submenu, you can print out your spectrum: To print your spectrum, do the following:

---Integrals: select "Scaled, Horiz", this is to show your integration underneath each peak.

---Peak frequencies: select "On peaks, var,ppm", this is to display the chemical shift on top of each peak.

---Click on **"automatic plot data**", your spectrum will be printed out.

14. Type "e" to eject your sample and put in the standard sample and type "I"
15. Exit