NMR

<u>You may find that useful information can be obtained from using the website:</u>

http://www.aist.go.jp/RIODB/SDBS/menu-e.html (or do google and SDBS)

click on "search compounds"

use compound name (try using different versions of the compound name because the website is kind of finicky about exactly how you name the compound) If you can't find spectra from your compound name then use the molecular formula portion and you will get a lot of molecules which has the same correct molecular formula. You can look through the list and try to find a molecule with the correct name. If you are not sure about the name if you click on the name you will get all spectra available for the molecule and also the structural formula for the molecule named.

(by the way the SDBS spectra give assignments for every single proton in the molecule.)

This handout was written by Dr. Juliet Hahn. No person was consulted in the writing of this handout.

WARNING: The NMR is a superconducting magnet. You should not get behind the yellow chains near the NMR with your wallet or you may wipe out credit cards. You should not get behind the yellow chain with anything metallic like watches, keys, coin money – you may seriously damage the brand new NMR (a $200,000 piece of equipment)

NMR collection : (in general if you left click over any button, the NMR will tell you what the button does)

1. after logging in, double click on the delta icon, turn on air

2. In the delta screen, click on the thing that looks like the magnet (the big shiny thing in the room)

3. The spectrometer control window shows up. Click on the sample button in the spectrometer control window and then in the sample window click on the eject (up arrow) button .

4. **This step is very important. If anything goes wrong to damage the spectrometer this is usually where people mess up the spectrometer. Remember big $$$. Be very careful**. Place your sample in the sample spinner and level the sample on the spinner. Take your sample over to the magnet and open the dust cover and gently float the sample and spinner into the air stream and let go. (take off any jewelry, watches, credit cards, wallet before going near the magnet)

5. In the sample window, click on the insert (down arrow) button.

6. Click on the autolock button and wait until it tells you that it has autolocked. (goes from yellow to green and tells you "locked") (You will get a better quality spectrum if you click on the gradient shim and lock instead but this takes a little more time.)

7. In the spectrometer control window, click on the experiment button. Under the global file, scroll down the experiments listed and click on **single pulse.ex.2**

8. Within the single pulse experiment window select autogain. Rename the file with a name of your choice – I suggest your initial and last name, your notebook experiment #, & date. (example: JHahnIV.26-2-25-08). Write down whatever comment you want to give. "…I had fun running the NMR today. I liked the little sample hovering thing….etc. " Press submit & go & OK.

9. When the experiment is complete, click on the octagon with cross sign to get peak numbers. In the menu inside the NMR screen, click on zoom and select the regions you want to print out.

10. Select integral in the tool bar and choose the integral icon. Create one big integral from one end to the other.

11. Print NMR by clicking on the printer icon.

Dr. Hahn
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