Instructions for the Bruker 400 MHz NMR

NOTE: Only students who have been properly trained in the use of the Bruker 400 are permitted to use this instrument.

1. Log into NMR computer and click the TopSpin icon.
2. Create a new datafile by typing `edc .`
3. *Insert sample:* `ej` to eject the standard; `ij` to inject your sample.
4. *Lock:* If your sample is in the same solvent as the previous one, it should lock automatically. If not, type `lock cdcl3` to lock on the deuterium signal; for other solvents, type `lock` and pick from the menu.
5. *Shim:* Type `topshim 1dfast .`
6. *Set up the spectrometer:*

`rpar PROTON all`	read in all ^{1}H parameters
`getprosol`	read in probe and solvent parameters
`ns 4 ; ds 0`	reduce the number of scans

(7. *Tune probe* if doing a non-H nucleus: `atma .`)

8. *Acquire Data:* Return to the main window and type:

`rga`	autogain (For ^{13}C and other weak nuclei, type `rg 200` instead).
`zg`	zero old data and get new data.

⇒ At this point, you may process your data on the console (steps 9–10) or using iNMR. If you use iNMR, skip to step 11.

9. *Process the data:*

`efp`	weight and transform the FID; apply phase correction from previous spectrum ("Exponentially multiply, FT, Phase")
`apk`	auto-phase the data

(For the next steps, be sure to save changes before returning to the top level: -button.)

Use the buttons of the Process tab to:

action	button	
phase		drag up/down on "0" and "1" in toolbar
set the reference ("calibrate axis")	0	click reference peak
peak pick		box the peaks to pick them
integrate	∫	drag over regions to integrate

10. Enter the printing/layout editor by typing `plot`. Use buttons to position the spectrum, expand it, create insets, etc. When it looks good, click the Printer button.

11. Replace the standard and verify that it has locked.
    (If you were using a solvent other than $CDCl_3$, this will require typing `lock cdcl3` .)

12. Close Topspin and log off the computer. Do NOT turn of the computer.

    ⇒ If you have a research account on the NMR Computer and wish to process your data using iNMR, you can access it from the ChemClub computers using SSHFS:

    (*i.* If this is the first time you are connecting from a given computer, you must use SSH first. In the Terminal program, type `ssh` *username*`@nmr400 true` , then respond "yes" to the confirmation query.)

    ii. Click the SSH icon on the dock, and enter the following:

Server:	nmr400
Directory:	/spectra
Password:	password for your research account (*username*)

    iii. A folder should appear on the desktop, within which you can navigate to your data just like you did in Organic. If it does not, verify that "Connected Servers" is checked in the Finder preferences.