

General Information About MestRe-C

MestRe-C is a program for the analysis of NMR data. With it, you will be able to expand regions of your spectra, reintegrate your spectra and perform other potential useful tasks. The program itself is part of the student image and should be available on any Windows computer on Truman's campus. Your instructor will let you know where you will be able to find your data files. The data files are typically in a folder named according to the date the experiment was run containing numbered subfolders. You can match the EXPNO printed on your hard copies of your spectra with the appropriate folder number. In your subfolder you will find several data files for that particular experiment.

General instructions:

- 1) Launch MestRe-C (All Programs:MestRe-C)
- 2) Know which folder your FID is in (look at EXPNO on your hard copy)
- 3) From the File Menu
 - a. Open (make sure it says Bruker XWIN-NMR)
 - b. Select the file called FID in your folder
- 4) From the Process Menu
 - a. Fourier Transform
- 5) Everything else can be done using the icons in the tool bar below the menu. For example:
 - a. Set the reference using the tool labeled TMS.
 - b. Use the Expand Tool (magnifying glass) to zoom in on a certain region.
 - c. Integrate a signal using the Integrate Tool (far right hand side of the tool bar)
 - d. Play around with it until you figure it out!

Things to pay attention to:

There should be a signal for TMS in your spectrum. If it is not at zero, set it zero in step 5a above. If you don't think you see TMS, talk to your instructor.

Your spectrum contains deuterated solvent, but no deuterated solvent can be 100% free of protons. Therefore, you will have some residual proton signal from your solvent. In the carbon spectrum, you will see a signal for the carbon(s). So, you need to know which signal(s) is/are due to your solvent. Refer to the table below to find the solvent in your spectra – then ignore it! Of course, a solvent peak may overlap with a “real” peak, so be careful.

Chemical shifts of common NMR solvents:

	¹ H-NMR	¹³ C-NMR
chloroform-d	7.25 (singlet)	77.0 (triplet)
acetone-d6	2.05 (singlet)	29.8 (septet) and 206.5 (poorly resolved septet)

Your spectrum may be contaminated with impurities, particularly if the NMR tube was not clean and dry when you added your sample. Common impurities include acetone (see chemical shifts in the table above) and water (chemical shift varies considerably).

More Detailed MestRe-C Software Directions

How to Transform and Customize your 1D NMR spectrum

Some MestRe-C Quirks/Helpful Items

A) Save your modifications as something else. Don't write over your FID.

Ex:

- Save As
- QEEB.transformed

B) MestRe-C generally has modes (Zoom mode, Integration mode, etc.). You may need to exit a mode in order to perform your next function. Press ESC to exit a mode. Supposedly you can undo with ESC but this has not been observed.

C) If you mess up, the only known way to undo your work is to close the spectrum and open it again.

Below is a *basic* guide to MestRe-C.

Getting Started

1. Start up MestRe-C by double clicking on the icon. It can be found in the "U Drive" Science area in Dr. Nagan's folder.
2. Open the file by going to:
 - File
 - Open
 - Choose your fid file under the appropriate experiment number. All of your FIDs are stored on the "U Drive", in SC\Patterson, then arranged by date and experiment number (both found on the printout of your spectrum).

Fourier Transform/Phasing

3. You need to carry out some FID processing.
4. Fourier transform and autophase the FID by going to:
 - Process
 - Fourier Transform

Zoom

5. Zoom in on a peak that you would like to integrate by going to:
 - Magnifying Glass Tool in your tool bar
 - Select the region you would like to enlarge with your mouse by left-clicking on the mouse and dragging the cursor from left to right – the region will be highlighted with a dotted box. You don't have to select the height of your box.

NOTE: To get back to the full spectrum, click on the full spectrum icon in your tool bar.

Setting the Chemical Shift Reference

6. Look for the deuterated solvent peak (actually some of the Ds have exchanged with Hs and so you see a peak). For CHCl_3 , it is a singlet and should be ~ 7.27 ppm. If you used a different solvent, you will have to look up the appropriate reference value.
7. Zoom in on the general region (like step 5).
8. Click on the apex of the peak.

9. Select the appropriate solvent and reference δ .

Integration

10. Zoom in on the region you want to integrate so that you can see the beginning and ends of the peaks.
11. Go to:
 - Process
 - Integration
 - Integrate
12. Choose a peak to integrate by left clicking on the mouse and dragging the cursor over the base of the peak.
13. Continue selecting peaks to integrate until all peaks have been integrated.
14. You can scale your integration by right clicking on a peak and typing in a number.

Peak Picking

15. If you would like the peak labels to be on the screen, go to:
 - Tools
 - Peak picking
 - Options
 - Show Peak Picking on Screen
16. To see the chemical shift values for all peaks above a certain threshold, go to:
 - Tools
 - Peak picking
 - Peak picking
 - Left click and drag horizontally across peaks to be picked.
17. To measure a coupling constant you can either do it through peak pick or you can manually do it through:
 - Tools
 - Measure Coupling Constants
 - Click on the two peaks that you want to measure J

Inset Expansion Spectra

18. Zoom in on peaks to be shown in the inset.
19. Go to:
 - View
 - Create Expansion
20. Click on full spectrum tool to see the whole spectrum.
21. Move axes and spectra to desired positions by:
 - Move the cursor over the axis or spectrum until a hand is shown.
 - Left click and drag to the desired position.