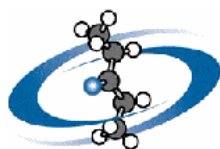




# Chemistry Department

## NMR/Instrumentation Facility

*Prepared by Leila Maurmann*



ACD/Labs  
NMR Processor

## NMR DATA PROCESSING

---

This manual is intended as a guide to NMR data processing using ACD/Spec Manager software available to the users of the NMR facility:

### Requirements:

- licensed version of ACD/Labs (available with NMR lab manager)
- Windows 2000 or XP operating systems
- minimum of 512 MB of RAM memory
- CD-ROM drive

### Retrieving data from NMR instruments

From the 200MHz:

- use an FTP software to download data into your computer (ask manager for IP address)

From the 400MHz:

- use a pen drive
- use an FTP software to download data into your computer (ask manager for IP address)

The folder loaded into your pen drive or from FTP should have a **fid** extension:

*filename.fid* (filename=saved data name) containing four files: fid, log, propar and text.

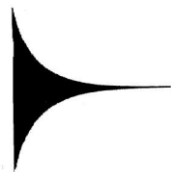
## Processing with ACD/Spec Manager NMR Processor

---

Word/phrase in square brackets [ ] are icons that can be accessed by a left mouse button click

This guide can be used to process NMR data using the ACD/Lab software version 10.

1. open ACD lab software
2. on the ACD/Spec Manager:
  - a. click **[OK]** and select folder desired (*filename.fid*)
  - b. double-mouse-click on *filename.fid* and check for the 4 files: fid, log, propar, text
  - c. select fid (it will be highlighted)
  - d. click **[Open]**
3. you will see the FID on the ACD screen:



4. check the spectrum parameters:
  - a. on top toolbar **[View]** - **[Spectrum Parameters]**
  - b. check the parameters list: original points count
  - c. close window

## Fourier Transform

---

5. the ACD toolbar for processing is composed of the following icons:  
**[ZeroFilling]** **[FIDShift]** **[LinearPred]** **[Wfunctions]** **[Fourier Tr.]** **[Apodization]**
6. click on **[ZeroFilling]**:
  - a. on the window increase the points count to a larger number than the acquired original points count, e.g. 31375 (from  $^{13}\text{C}$ ) to 32768 or 13103 (from  $^1\text{H}$ ) to 16384 (typically  $fn=2*np$ , where  $fn$  is the point count for FT and  $np$  is the acquired original points)
  - b. click **[OK]**
  - c. observe the change in the FID (there will be a line at the end of it)
7. click on **[Apodization]**
  - a. you will see the frequency domain spectrum - i.e. peaks
  - b. the toolbar changes to:  
**[√]** **[X]** **[Apply FT]** **[Apply PC]** **[LinearPred]** **[WFunctions]**
  - c. you can change the window functions to increase signal to noise ratio:
  - d. click on **[WFunctions]** and change the window if desired, the options are: *exponential* (typical for 1D), *Lorentzian-Gaussian*, *TRAF Function*, *Sine Bell*, *Shifted Sine Bell*.
  - e. you can also directly change the **LB** (line broadening) of an exponential using the LB arrows on the toolbar

8. click on [\[LinearPred\]](#)
  - a. used to remove artifacts and distortions
  - b. select Backward check box and change the values to:
    - i. points to predict - 1 - 2
    - ii. base points - 5 - 512
    - iii. coefficient count - 32
  - c. click on [\[Apply\]](#)
9. click on [\[√\]](#) or [\[X\]](#) to finish Fourier transform or to return to FID

## Analysis

---

10. the toolbar will change to:  
[\[PhaseCorr\]](#) [\[BLine Corr\]](#) [\[Peak Picking\]](#) [\[Peak Fitting\]](#) [\[Integration\]](#) [\[Reference\]](#)  
[\[Annotation\]](#) [\[Multiplets\]](#) [\[Assignment\]](#)
11. click on [\[PhaseCorr\]](#)
  - a. toolbar changes to:  
[\[AutoSimple\]](#) [\[Auto BL Opt\]](#) [\[Auto Symm\]](#) [\[Mouse Ph\]](#) [\[Fine Tuning\]](#) [\[Options\]](#)
  - b. you can use the arrows to change **ph0** and **ph1**
  - c. or click on [\[Mouse Ph\]](#) and with the left-mouse-button move peaks up and down to adjust the phase
  - d. [\[Auto Simple\]](#) works well for 1D spectra
12. click on [\[BLine Corr\]](#)
  - a. toolbar changes to:  
[\[Auto\]](#) [\[PeakLevel\]](#) [\[Peak by Peak\]](#) [\[Clear\]](#) [\[Options\]](#)
  - b. click on [\[Peak Level\]](#) and take crossline to level desired in the spectrum and left-mouse-click to set threshold
  - c. the chemical shifts will appear on each peak
  - d. click on [\[√\]](#) or [\[X\]](#)
13. click on [\[Reference\]](#)
  - a. toolbar changes to:  
[\[Auto\]](#) [\[Clear\]](#) [\[Options\]](#)
  - b. on [\[Options\]](#) select reference desired: TMS or solvent (if you had the correct parameter on you spectrum acquisition, the corresponding solvent will appear on the “solvent list”
  - c. or [\[Auto\]](#) - [\[√\]](#) or [\[X\]](#)
14. click on [\[Annotation\]](#)
  - a. use it to label peaks
  - b. click on a peak and a window will open, type what the desired notation and click [\[√\]](#)
15. click on [\[Integration\]](#)
  - a. toolbar changes to:  
[\[Auto\]](#) [\[Manual\]](#) [\[Bias Corr\]](#) [\[Delete\]](#) [\[Clear\]](#) [\[Options\]](#)
  - b. use the mouse and click-and-drag around a peak to be integrated
16. click on [\[Multiplets\]](#)
  - a. toolbar changes to:

- [Auto] [J-Coupler] [Delete] [Clear All] [Options]
17. on the bottom toolbar click on **[Chem Sketch]**
    - a. you can draw your structure on the screen
    - b. on the bottom toolbar click on **[Processor]** to return to spectrum, a window will open and to add the structure to the spectrum select the “attach structure to the current spectrum” option
  18. click on **[Assignment]**
    - a. toolbar changes to:  
[By Peak] [By Region] [By Multiplet] [Clear]
    - b. click on atom number of the structure and a move towards the peak to which it is assigned to (you will see a **red line**)
    - c. the assignment will appear on the peak

## Report

---

19. saving as picture files
  - a. click on **[Edit] - [Copy to Clipboard] - [Spectrum]**  
open a word or power point file and paste spectrum
  - b. click on **[Edit] - [Create Report] - [Standard]**  
a ChemSketch file opens with the standard report template, you can save the file in various formats: .cdx, .pdf, .bmp, .gif use **[File] - [Save As]**
  - c. click on **[Edit] - [Export Report to PDF] - [Standard]**  
saves files in .pdf format