

ACD Lab - Guidelines for NMR Processing – Chem 362

General Instructions

Open **2D NMR Processor** located on the desktop.

Choose **Cancel**.

Under the **File** tab, click **Open**, and then choose **From 1D NMR Directory**.

Choose **Files of type: Any File (*.*)** from the dropdown menu.

Open your saved file from the folder: T:\Chemistry\ChemLabs\chem362\yourname.

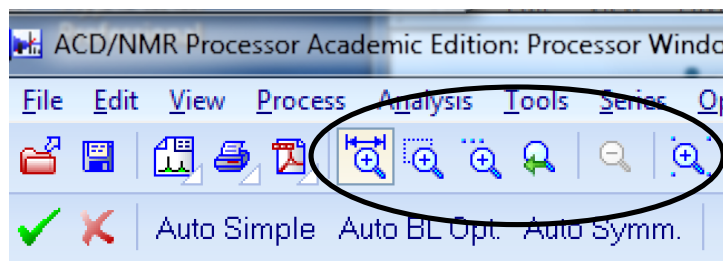
Choose the **fid** file and click **open**.

The fid will appear in the window. In the upper left corner, choose **Shortcut**. The prompt will ask if you want to view an informational video. Click **No**.

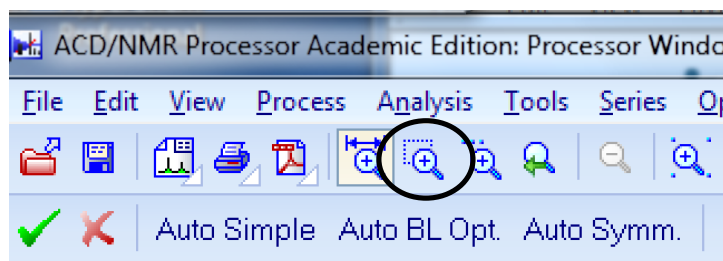
The processed NMR spectrum will appear in the window. A separate **Action Selector** window will also appear. Keep this window open. Each pull-down choice should read "Ask".

Phase Correction

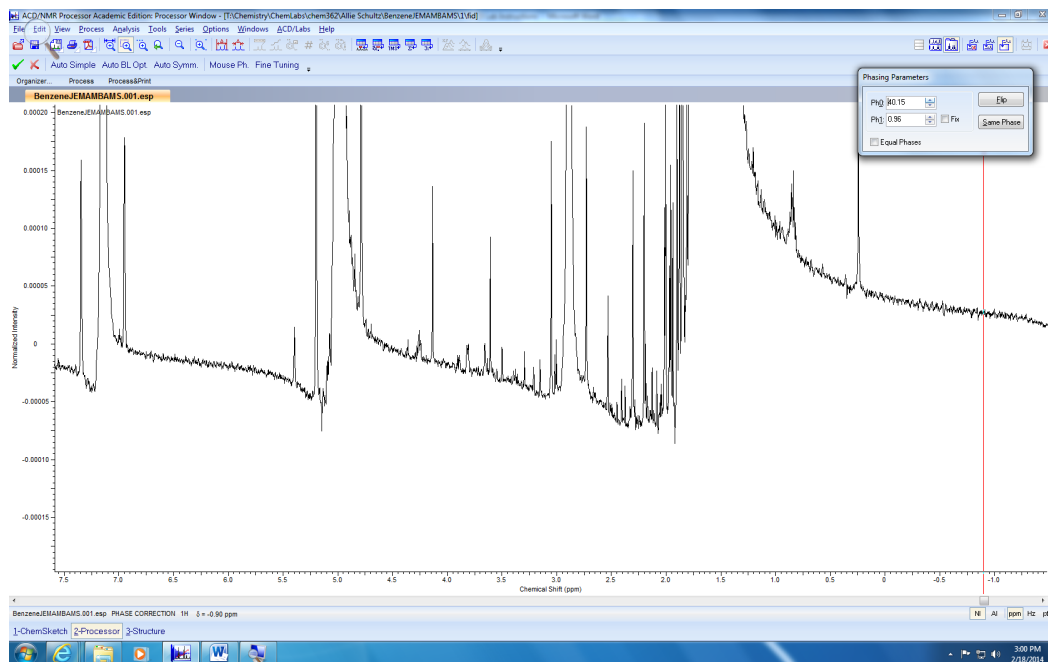
Begin by understanding the Zoom features in the program by using the tools shown below.



Set the zoom window to enclose the baseline of the tallest signal (approximately Y-Axis: 0.00020 to -0.00020, X-Axis: 8 ppm to -2 ppm) using the following tool.



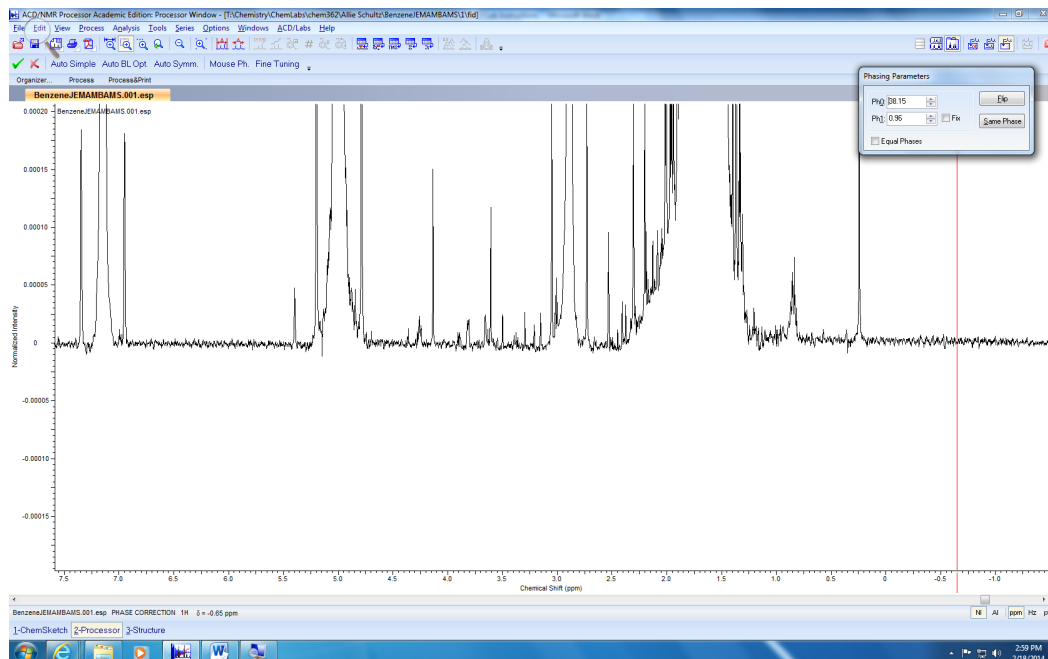
Your spectrum should look similar to the one below:



Click on the **Phase** button in the toolbar.

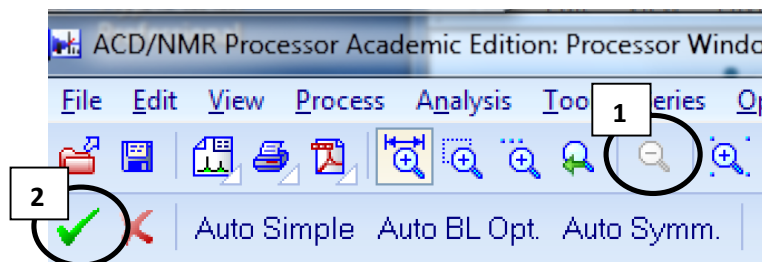
The **Phasing Parameters** window will appear. You will phase zero-order correction (Ph₀) and first-order correction (Ph₁).

Begin phasing the spectrum with Ph₀. This will automatically phase the tallest peak in your spectrum. In increments of 0.10, manually type values to change Ph₀ to make the baseline as straight as possible (see below).



If it is necessary to phase the other signals, do so by adjusting the Ph₁ value by a factor of 0.01.

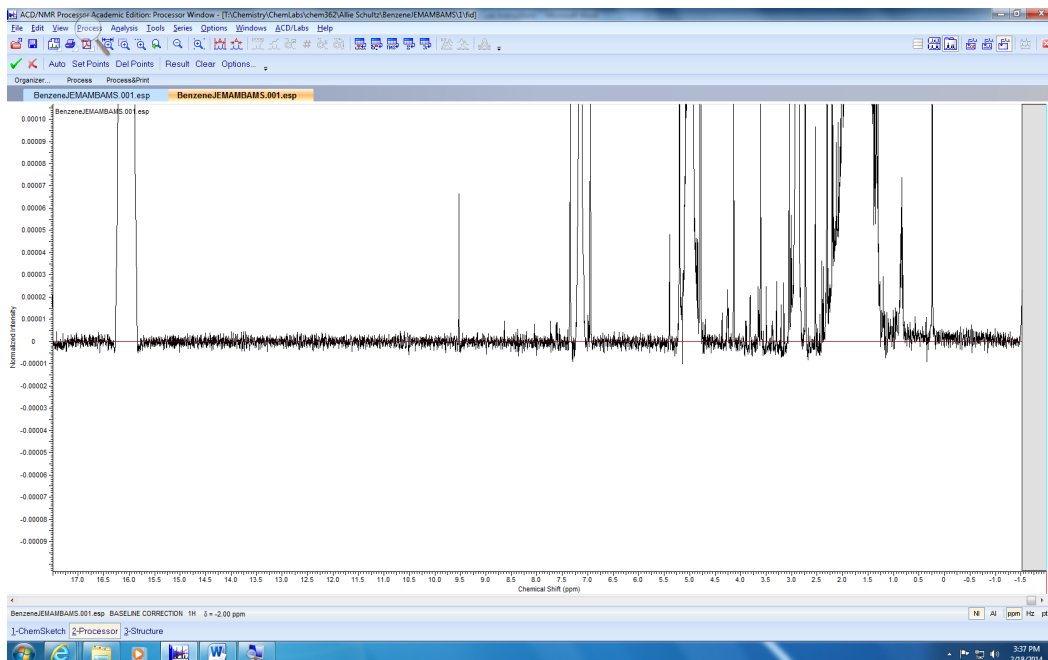
Zoom out (1), and then accept changes (2). This will exit the phase processor.



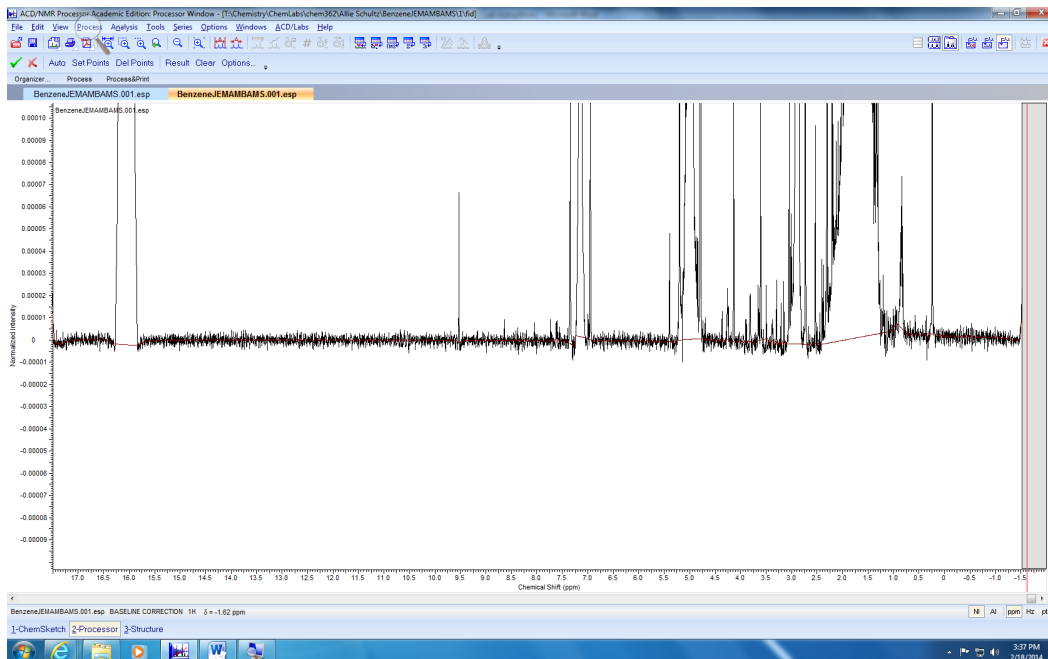
Baseline Correction:

For the baseline correction, set the zoom window to the approximate size (Y-Axis: 0.00010 to -0.00010, X-Axis: 18 ppm to -2 ppm) using the same zoom tool as before.

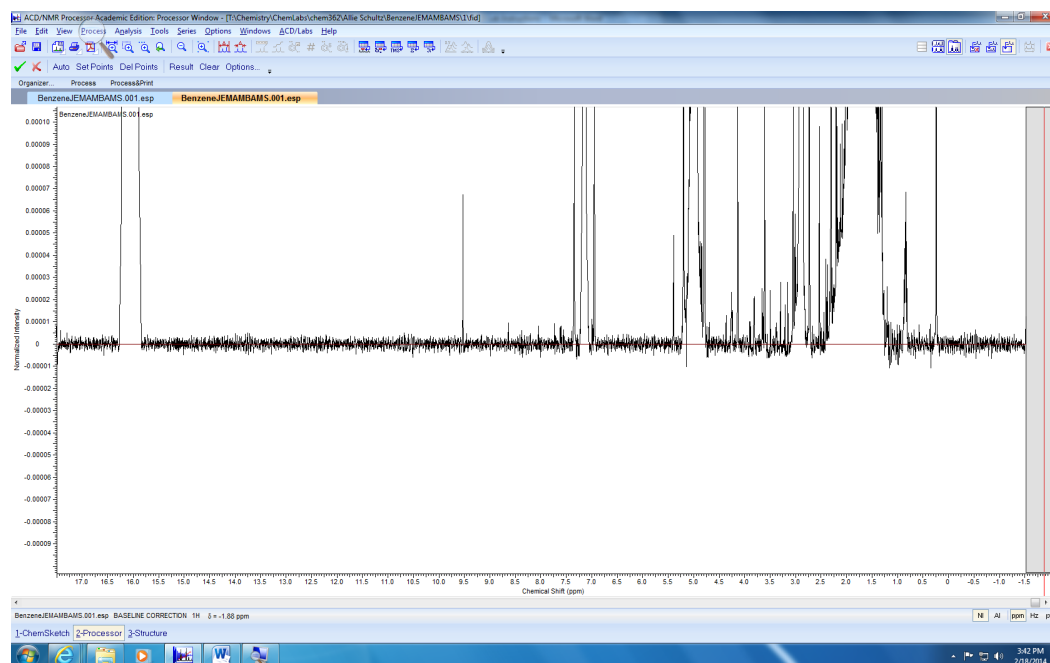
Click on **Baseline**. A horizontal red line will appear.



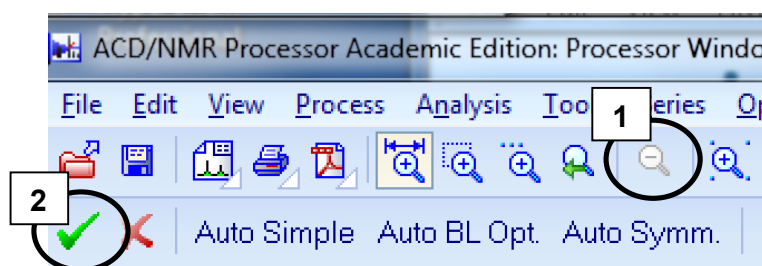
Click **Auto**. The window should look similar to the one below. Notice the red line is detecting a corrected baseline.



Click **Result**. You will see the corrected baseline as shown below.



Zoom out (1), and then accept changes (2). This will exit the baseline processor.

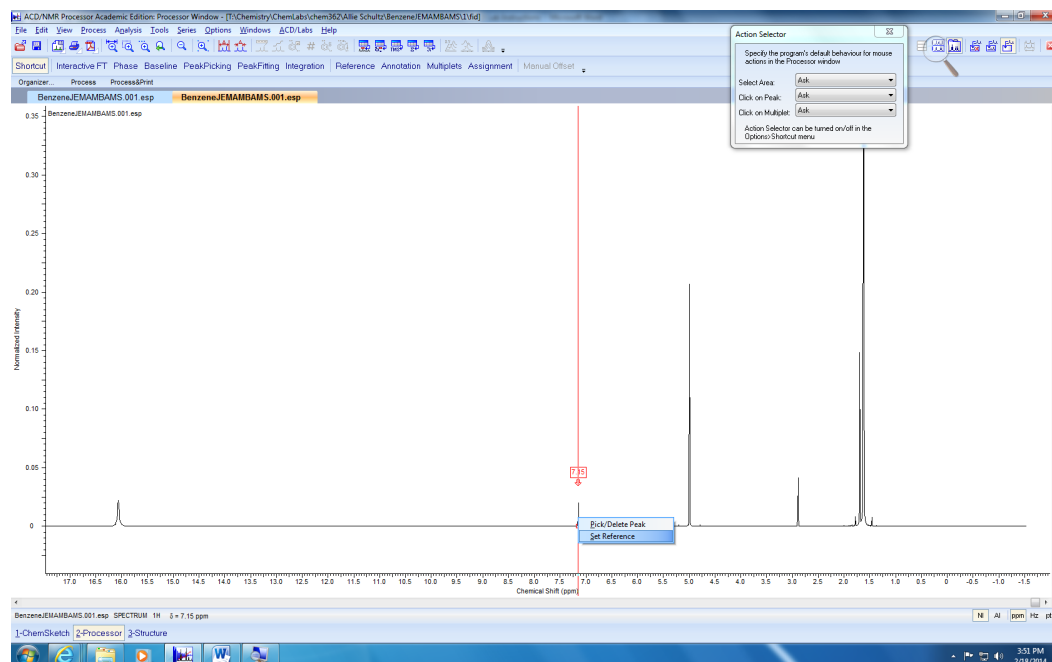


Setting the Solvent Reference

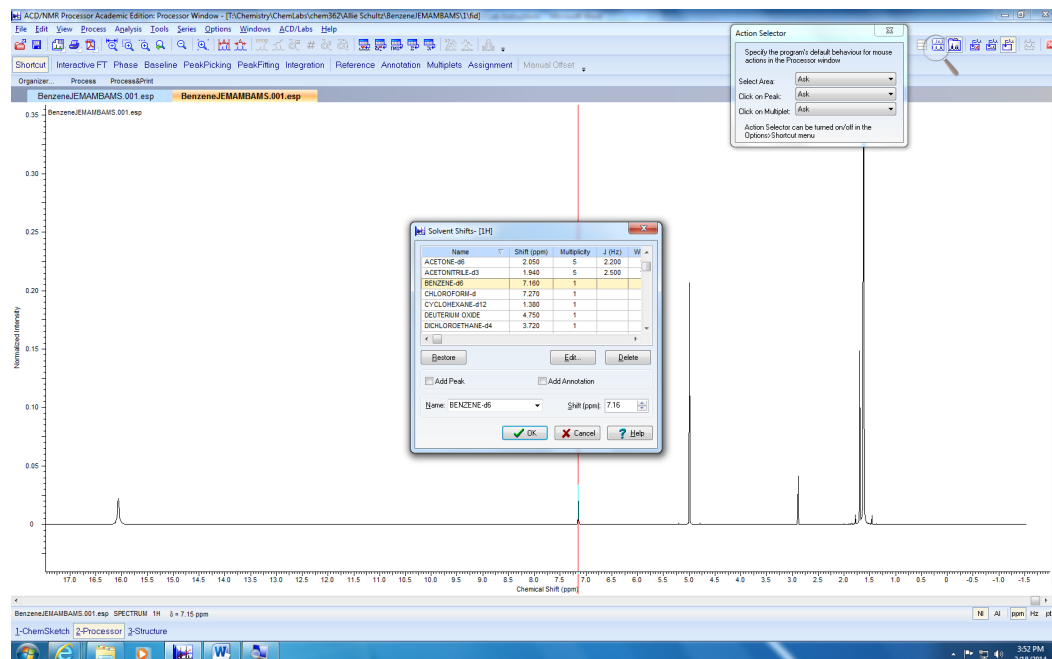
Be sure that the zoom tools are not highlighted.

Each deuterated solvent has a unique signal in the proton NMR spectrum. Hover over the solvent signal with the mouse (refer to the Appendix of your lab manual). Left click on the signal and choose **Pick/Delete** Peak. The spectrum will show the corresponding peak value (the signal for benzene in this example spectrum is 7.15 ppm).

Left click on the peak again and choose **Set Reference** (see below).



A window with a list of solvent reference values will appear. Choose the appropriate solvent you are using (see below). For benzene, the reference value is 7.16 ppm. Click **OK**.



Peak Picking and Integration

Be sure that the zoom tools are not highlighted.

To integrate a signal, align the red cursor to the far left side of the peak. Left click and drag the cursor to the far right side of the peak (Fig. 1). Choose **Define Multiplet and Integral** (Fig. 2). The corresponding peak value and integration will appear (Fig. 3).

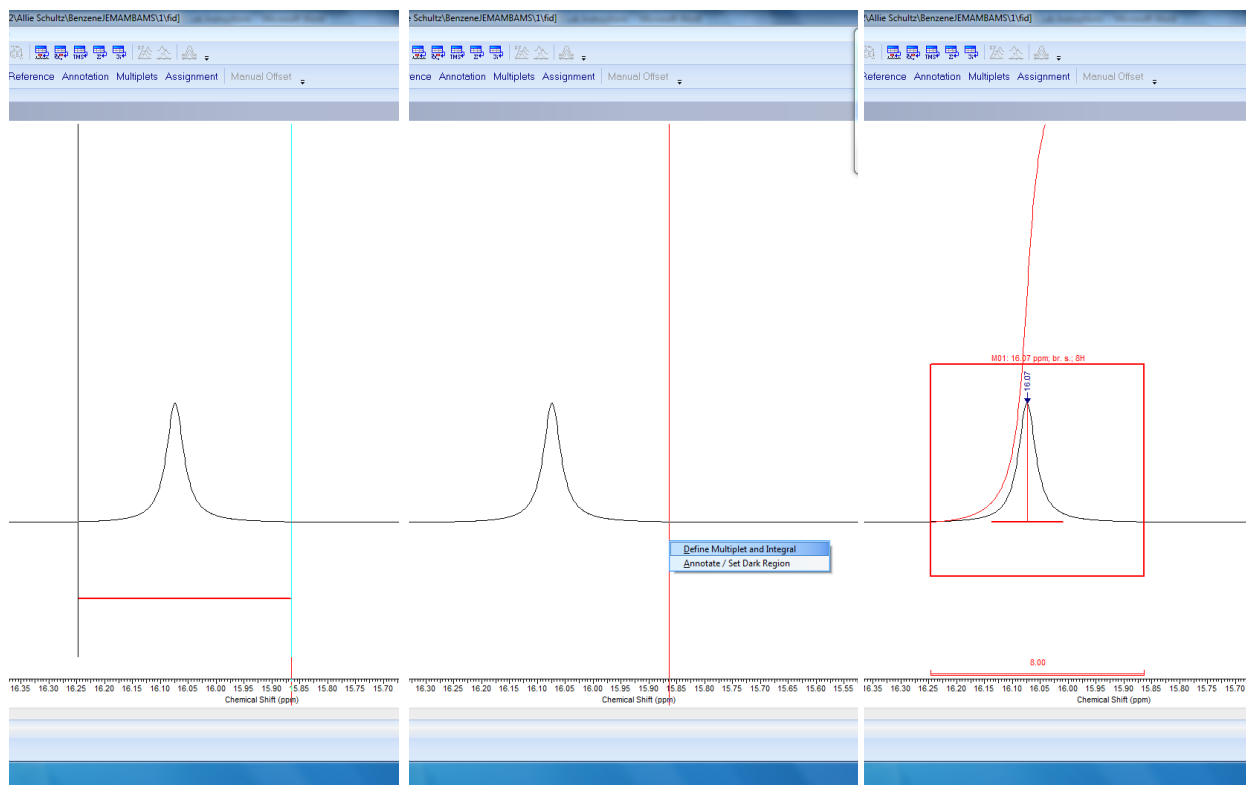


Fig. 1

Fig. 2

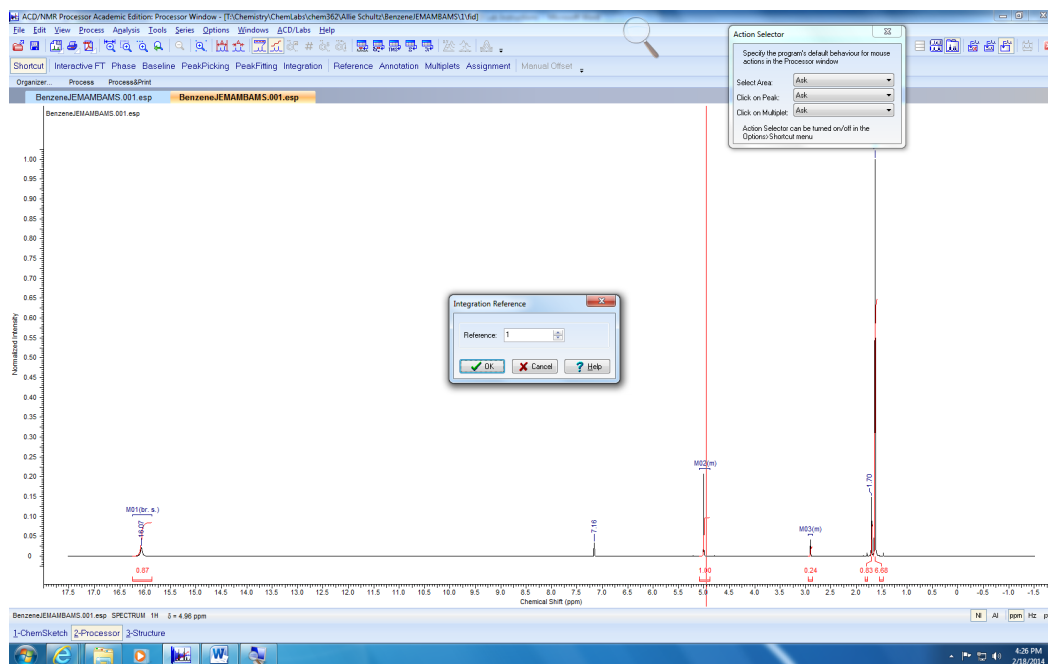
Fig. 3

Define the multiplets and integrals for each of the remaining signals as described above and zoom wherever necessary. Do not define the deuterated solvent peak.

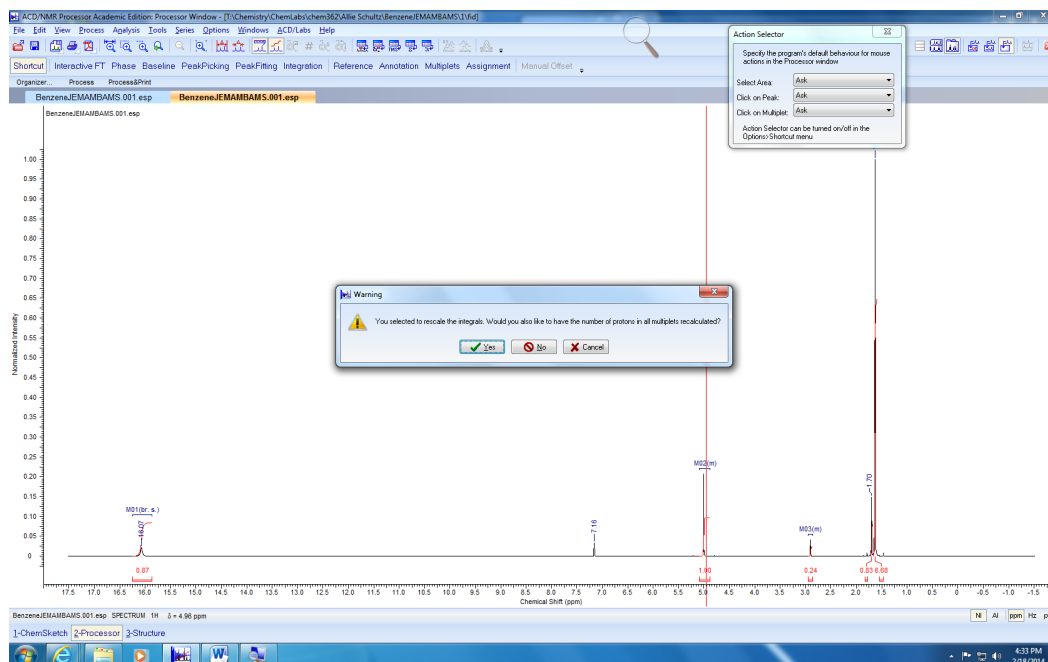
Setting the Reference Integral

Be sure that the zoom tools are not highlighted.

Choose the “ene” proton in the spectrum (hint: this signal will appear between 6–4 ppm). Left click on the integration value and a new window will appear (see below). Type the appropriate number of proton(s) to match the “ene” signal, and then click **OK**.



A new warning window will appear asking if you want to rescale the integrals for the rest of the multiplets. Click **Yes** (see below).



Creating a Report

Zoom out to view the entire spectrum. Choose **File**, **Print**, and **Standard**.

Follow the instructions to modify the parameters in each tab of the Print Menu.

Spectrum

Check **Whole Spectrum**.

Uncheck **Zoom Region**.

Tables

Uncheck **Table of Integrals**.

View

Uncheck **Vertical Scale Factor**.

Text

Check **Page Title**. Add your name here.

Check **Comment**. Add the name of the deuterated solvent you used here.

Choose **OK**.