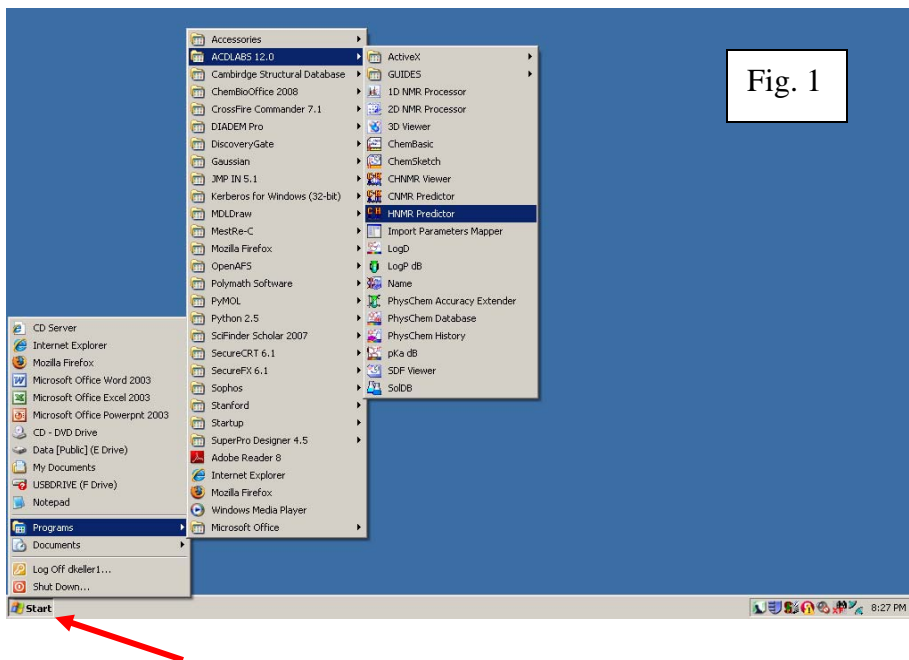


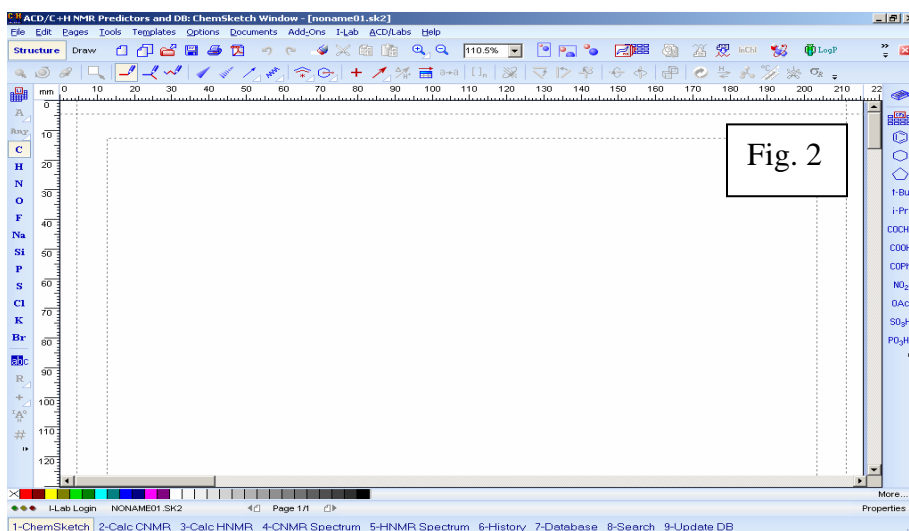
Table of Contents: ACD Tutorial

Page 1	Downloading and/or Launching ACD 12.0
Pages 2-6	Drawing a Molecular Structure
Pages 6-7	Predicting an H or C13 NMR Spectrum
Pages 7-8	Expanding the X-Axis of the Spectrum
Pages 9-10	Identifying Chemical Shifts and Coupling Constants
Pages 11-12	Changing the Default Frequency and Recalculating
Page 13	Predicting the Boiling Point of a Compound
Page 14	Generating an IUPAC Name for a Compound

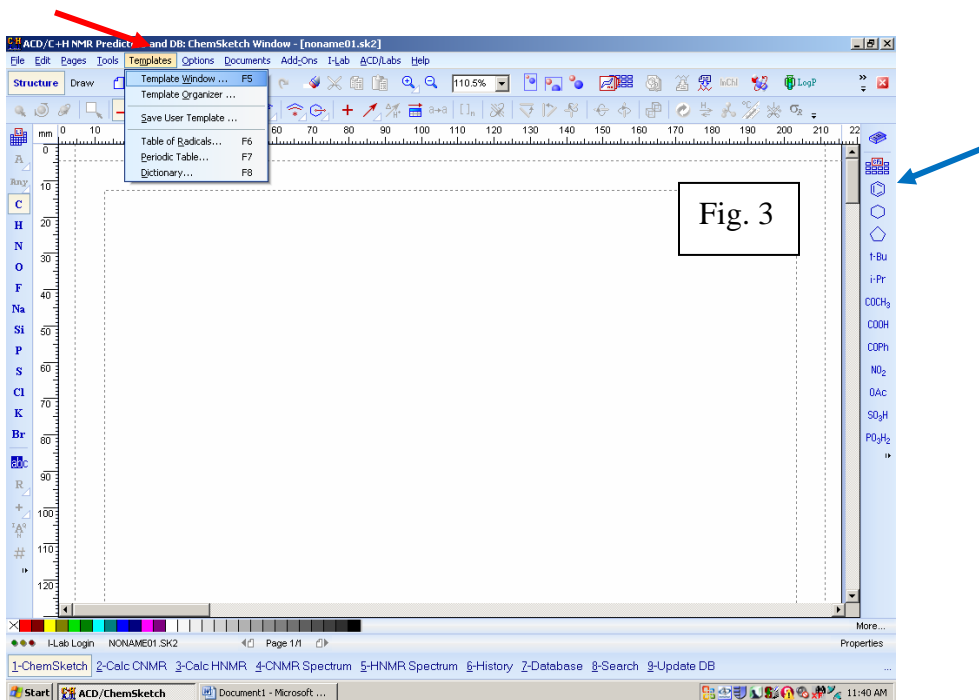
If you are on any of the computers in the Swain Chemistry Library, to launch ACD LABS 12.0, left click and hold the cursor on Start (red arrow below at lower left), and move the cursor to Programs, ACDLABS 12.0, and HNMR Predictor, as shown in Fig. 1. At the latter, release the click, to reach the screen shown in Fig. 2. If you are not in Swain, or are using your own laptop, you may have to first download ACDLABS 12.0 software, using the link reached from the Swain homepage, by clicking on “Software” [on the left hand side of the page], then clicking on “Download ACD software”.



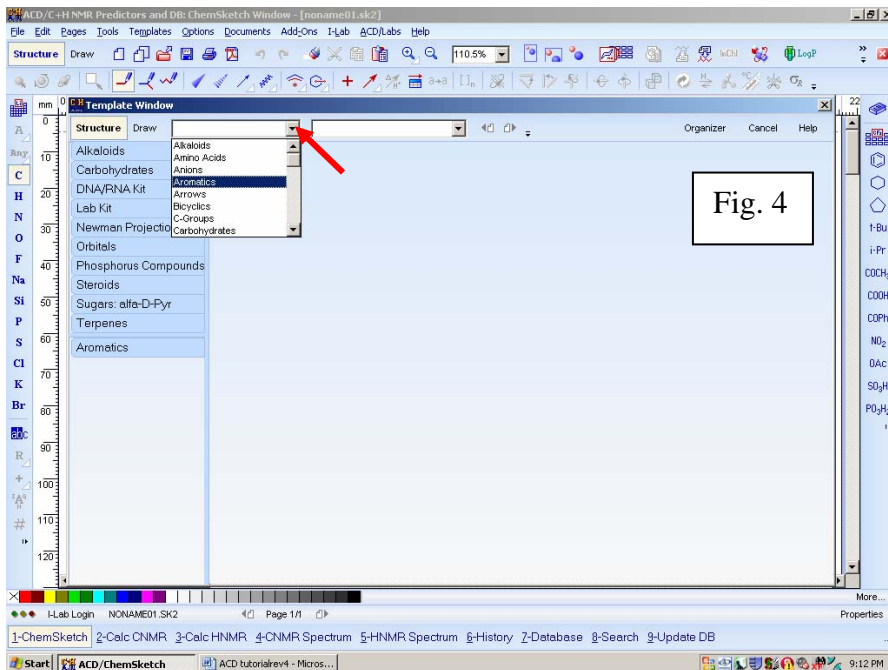
To predict the H NMR or C13 NMR spectrum of a molecule, or its boiling point, you need to first draw its chemical structure onto the drawing area (the blank area shown in Fig. 2). We will use toluene [methylbenzene] as an example, to predict its HNMR spectrum.

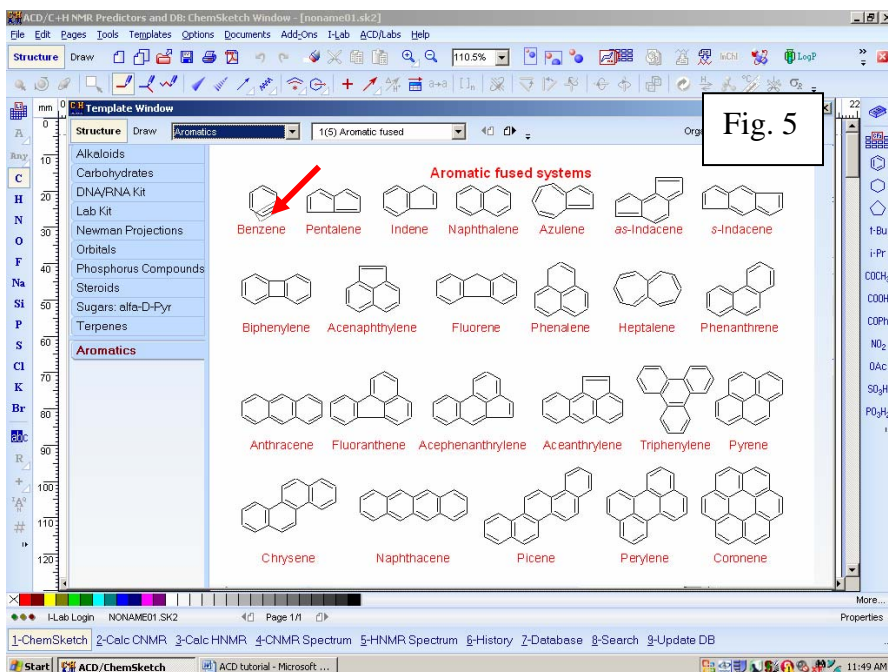


You can add a benzene ring to the drawing area in two ways. For the first way, left click on “Templates” (red arrow, Fig. 3). Then left click on “Templates Window” [just under “Templates”] to get to Fig. 4.

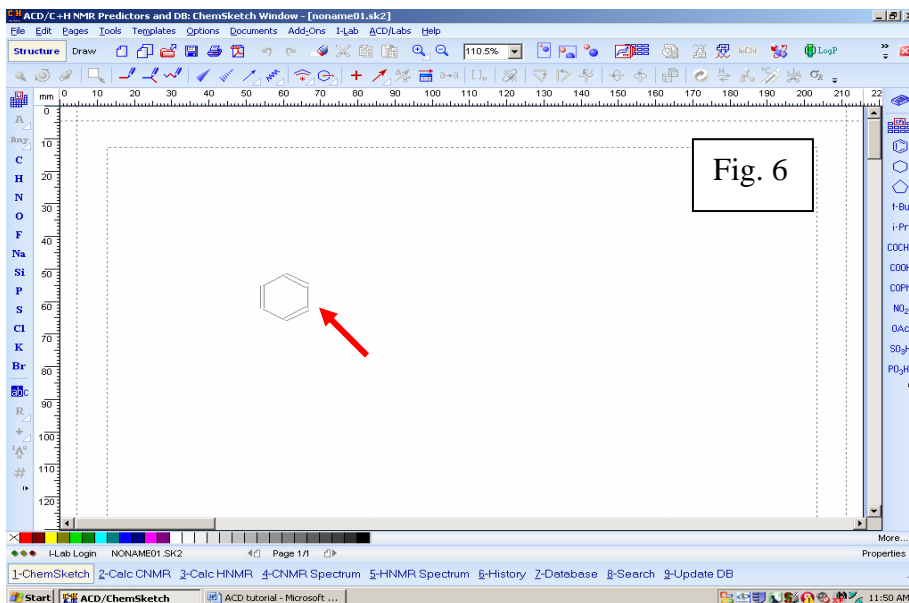


Left click on the down arrow (red arrow in Fig. 4). Then left click on “Aromatics”. You should see the screen in Fig. 5.





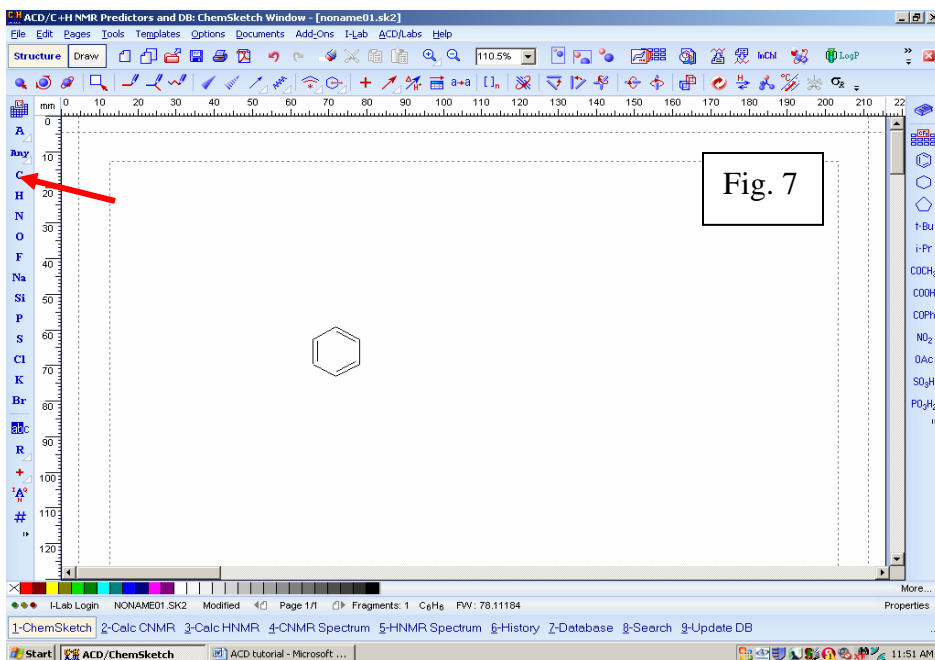
Left click on the benzene ring (red arrow, Fig. 5). You should then be able to move the cursor/ring anywhere on the drawing area, such as shown with the red arrow in Fig. 6.



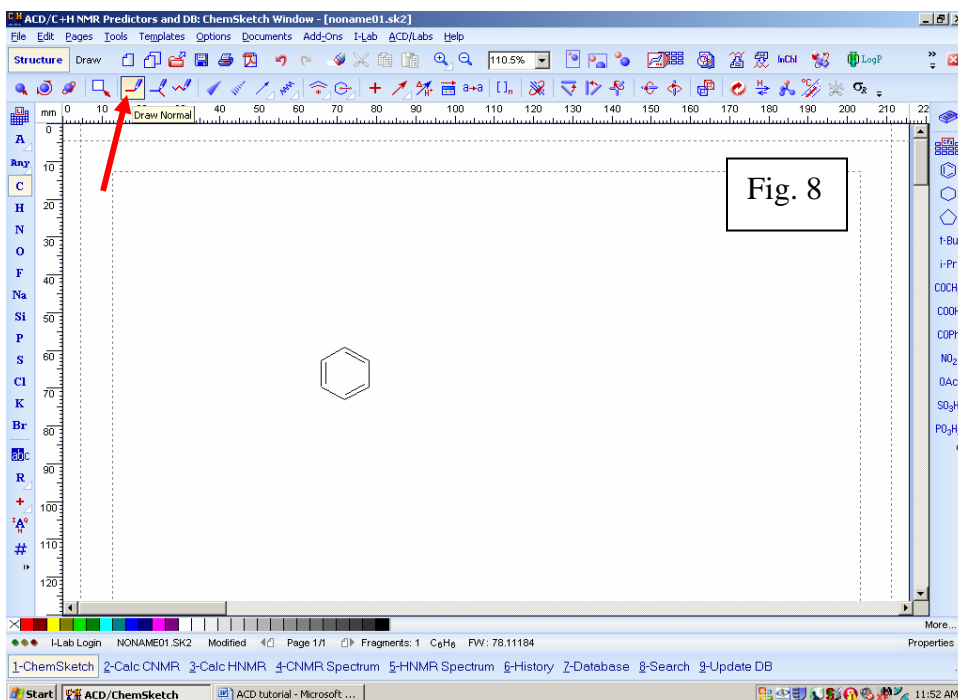
By left clicking on the drawing area, a benzene ring will be inserted where you clicked, as shown in Fig. 7. Don't click a second time, unless you want to add more rings.

Using the second way to add the ring, you could have clicked on the benzene ring [blue arrow, Fig. 3], and that would have taken you directly to Fig. 6, where you left click on the drawing area.

Instead move the cursor to the C (red arrow Fig. 7), and left click on it.

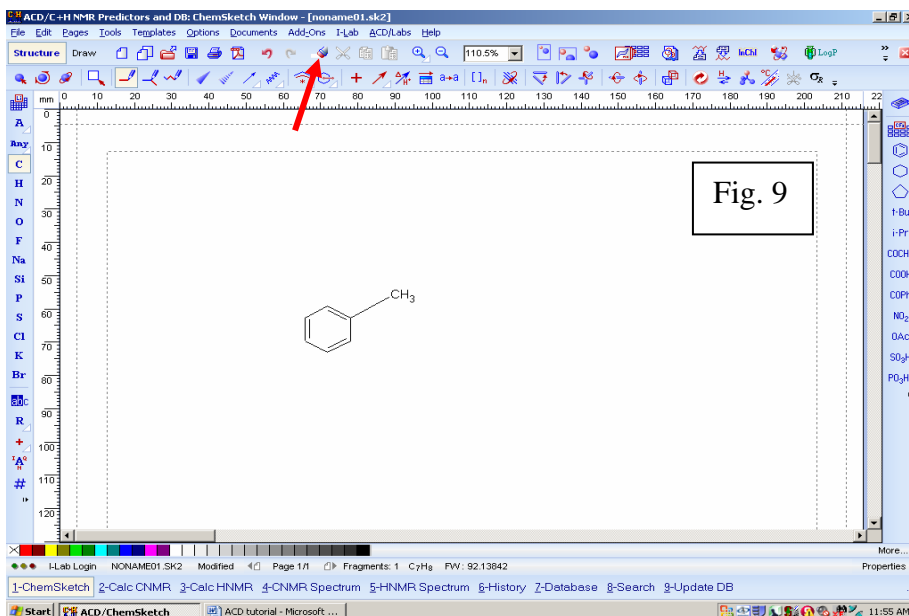


Observe that the single bond icon (red arrow in Fig. 8) is also highlighted when you select the C. This is the “Draw Normal” single bond. Other types are to the right.

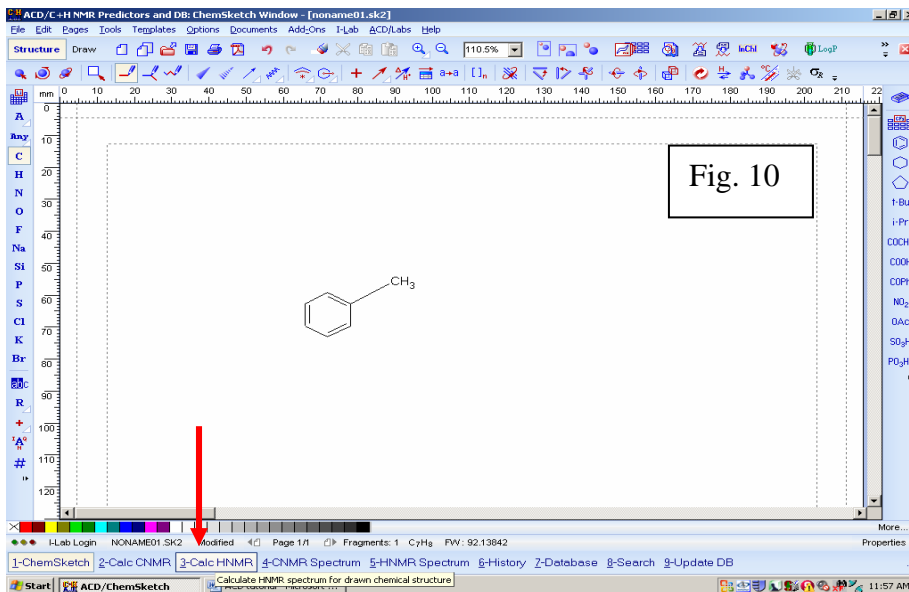


Left click near the benzene ring and drag to a C on the ring. This will add a CH₃ to the ring, as shown in Fig. 9. If you make a mistake you can erase with the eraser tool (red arrow in Fig. 9).

You can select other types of single bonds for stereo purposes etc. To add a double bond, just left click once on a single bond, or click twice to make it a triple bond. A third click converts it back to the single bond.



We now have drawn the toluene structure in the drawing area, and can use it to predict the HNMR spectrum. To do so, left click on the “3-Calc HNMR” (red arrow Fig. 10). Or left click on the adjacent “2-CNMR” to predict the C13 spectrum.



This will produce the spectrum shown in Fig. 11. The frequency used for this calculation was 400 MHz (the default value). We will later show how to change this, if desired.

The structure box can be moved to any location on the spectrum by left clicking and dragging it, so that it does not obscure any peaks.

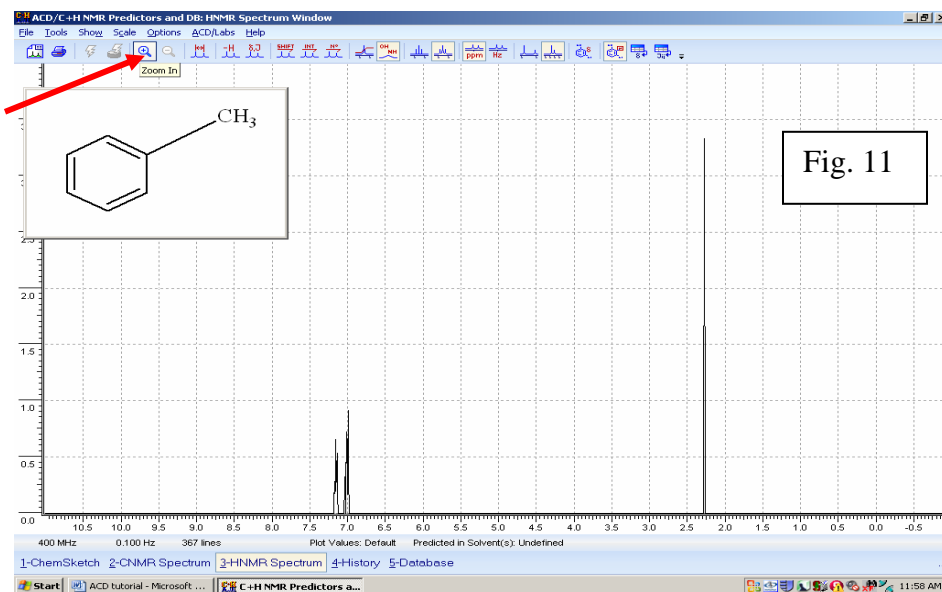


Fig. 11

Plotted on this scale it is often difficult to see the multiplicity in peaks, i.e., its hard to determine if there is a singlet, doublet, triplet, multiplet etc. To resolve this one can expand the scale for any given area as follows. Left click on the “Zoom In” icon (red arrow Fig. 11). Then move the cursor to the area where you want to expand the scale, and it will bring two intersecting lines to this location (see red arrow in Fig. 12).

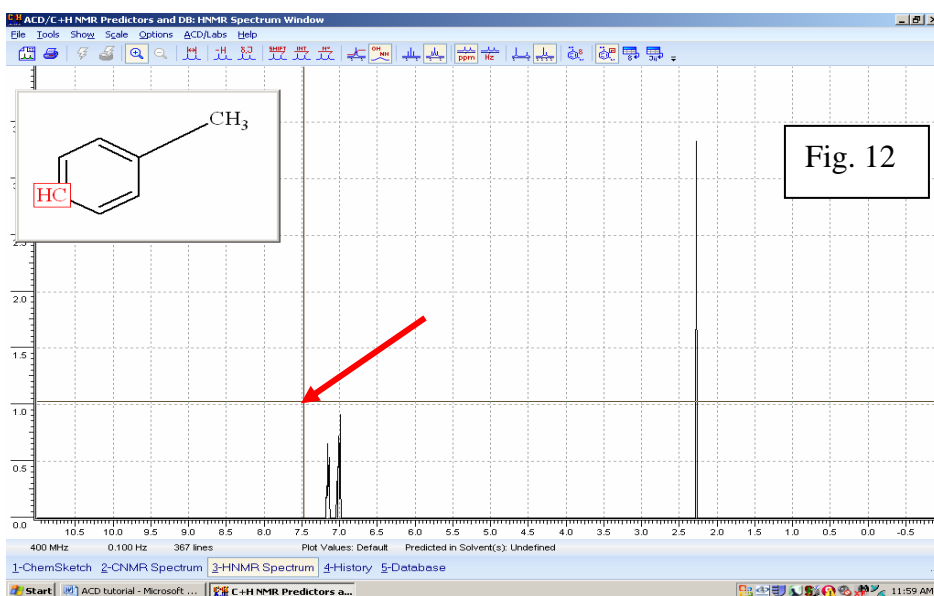
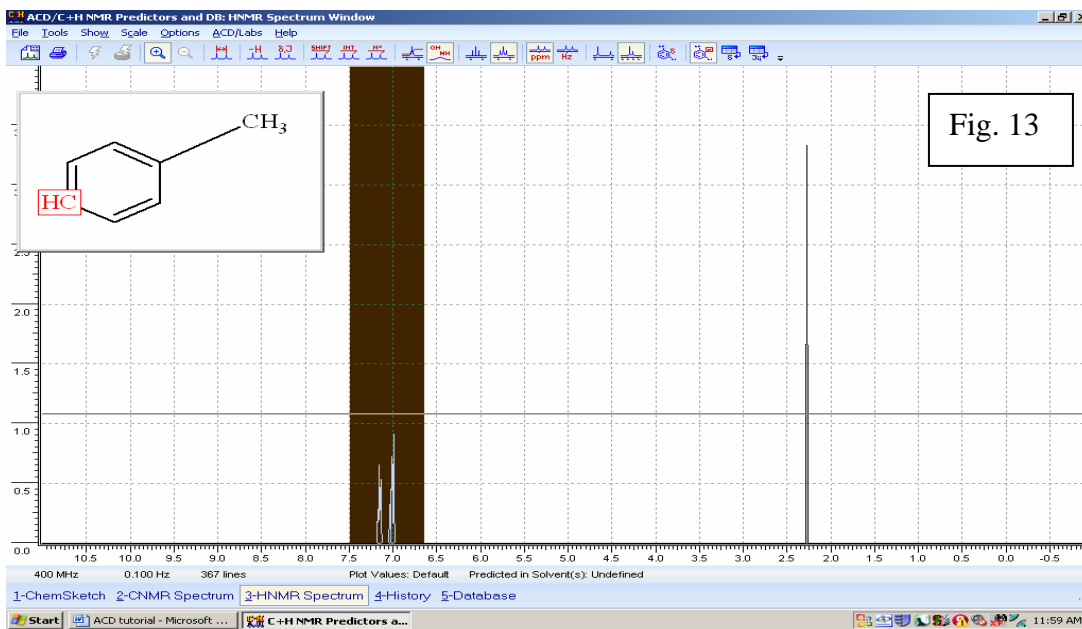
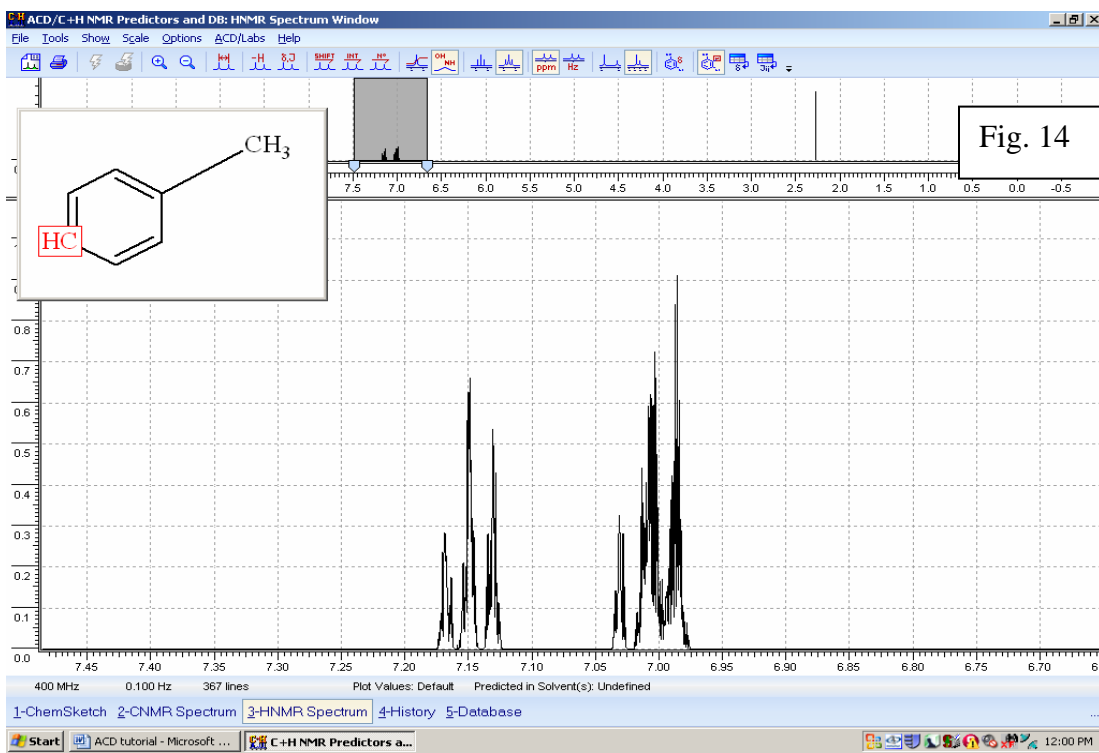


Fig. 12

Then left click and hold and drag the cursor to the right. As you drag, an area will darken, as shown in Fig. 13.



After you release the left click, the darkened area will show up with an expanded scale, as shown in Fig. 14. Also, at the top you can see the whole spectrum, and a shaded region showing which part of the spectrum has been expanded.



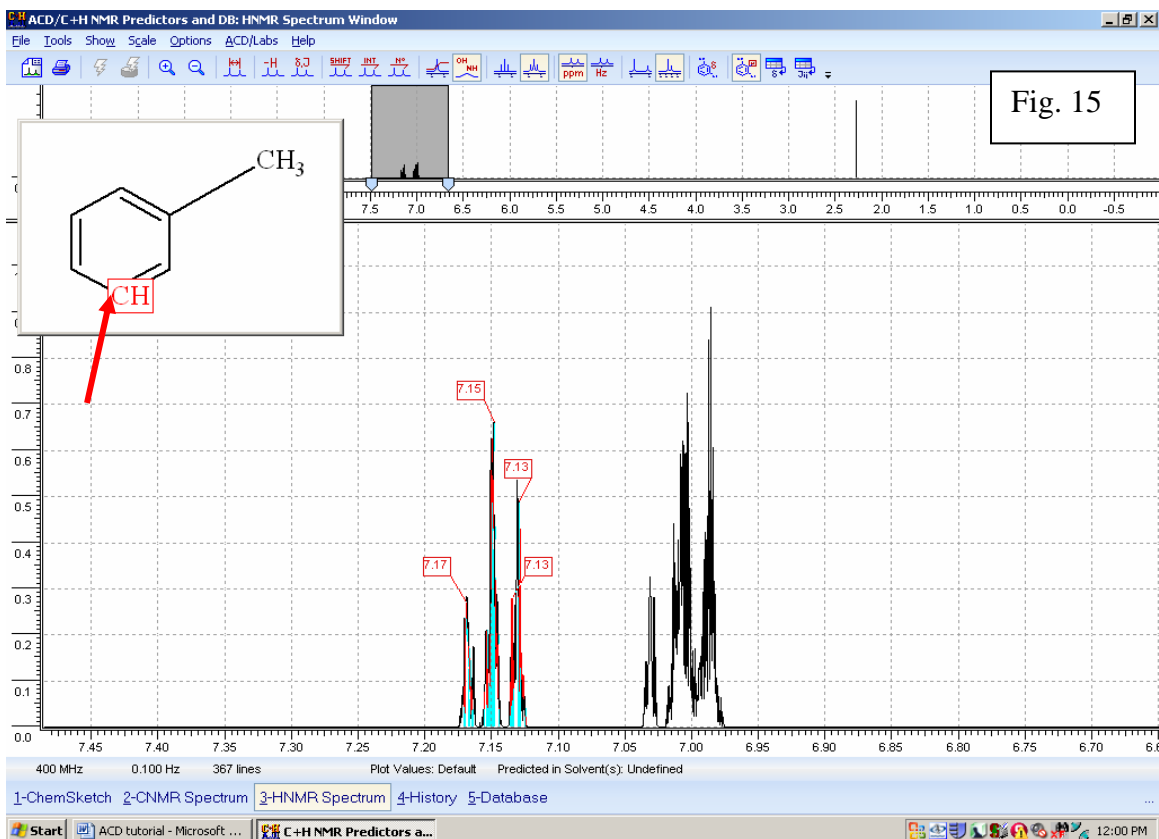


Fig. 15

Now, using the cursor, one can discover which peaks are connected to each of the H's. For example, if you place the cursor on the H shown with the red arrow in Fig. 15, you will see chemical shift values assigned to the peaks for that H [the numbers in red boxes near peaks]. You will note that since this H has a nearest neighbor H on either side of it, you would expect to see its peak split into a triplet using the $n+1$ rule [$2+1=3$]. And to a first approximation, that's what you do see. However, each leg of the triplet is slightly further split due to next nearest neighbor interactions, and next next nearest neighbor interactions etc, which could be seen more clearly if you zoomed in on this section even further. However, for this course you are not expected to go beyond next nearest neighbor interactions. Hence we will not expand the scale any further, but instead we shall discuss additional aspects of the chemical shifts, and also introduce the coupling constants as well.

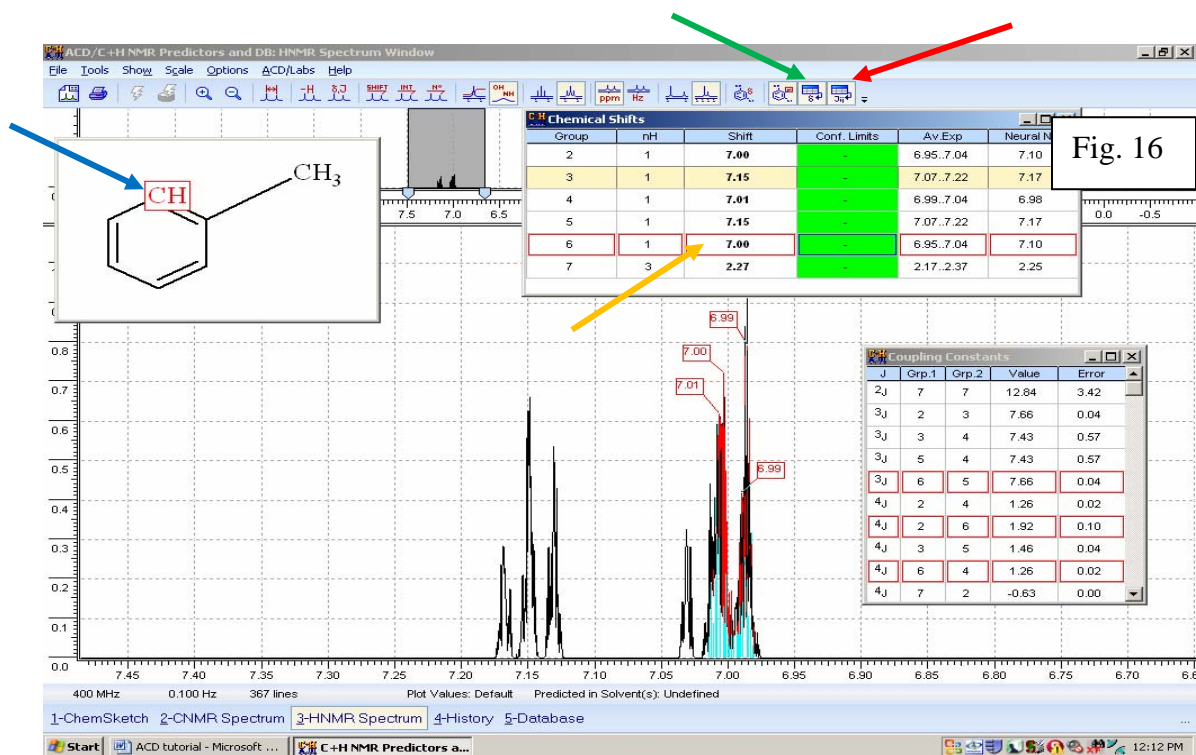
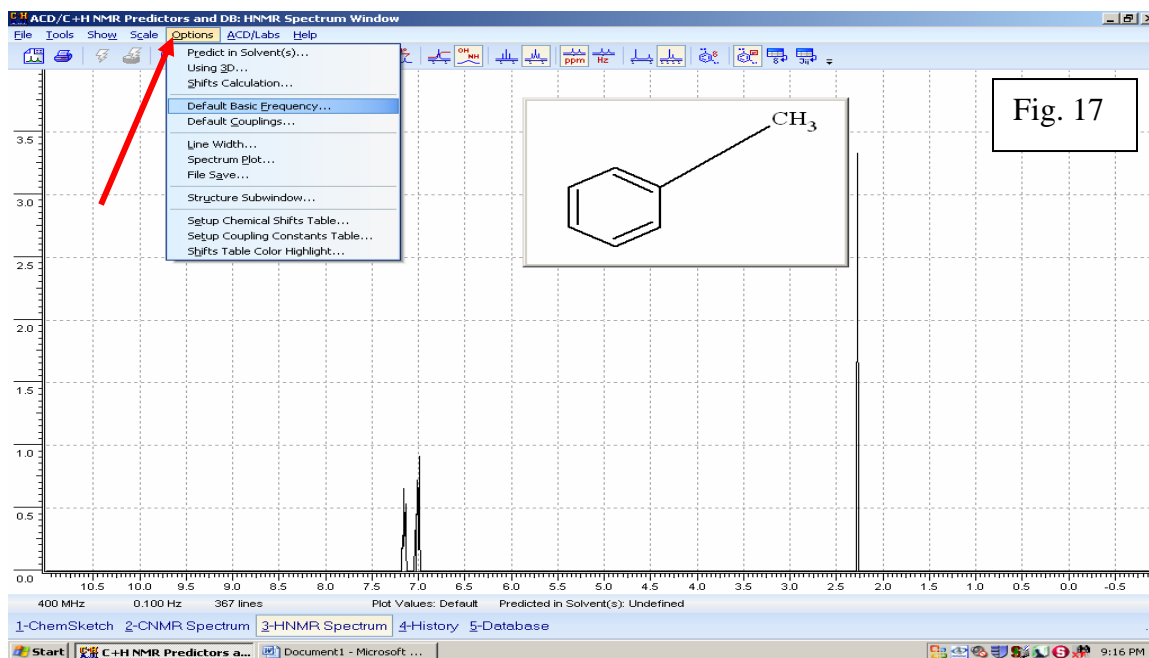


Fig. 16

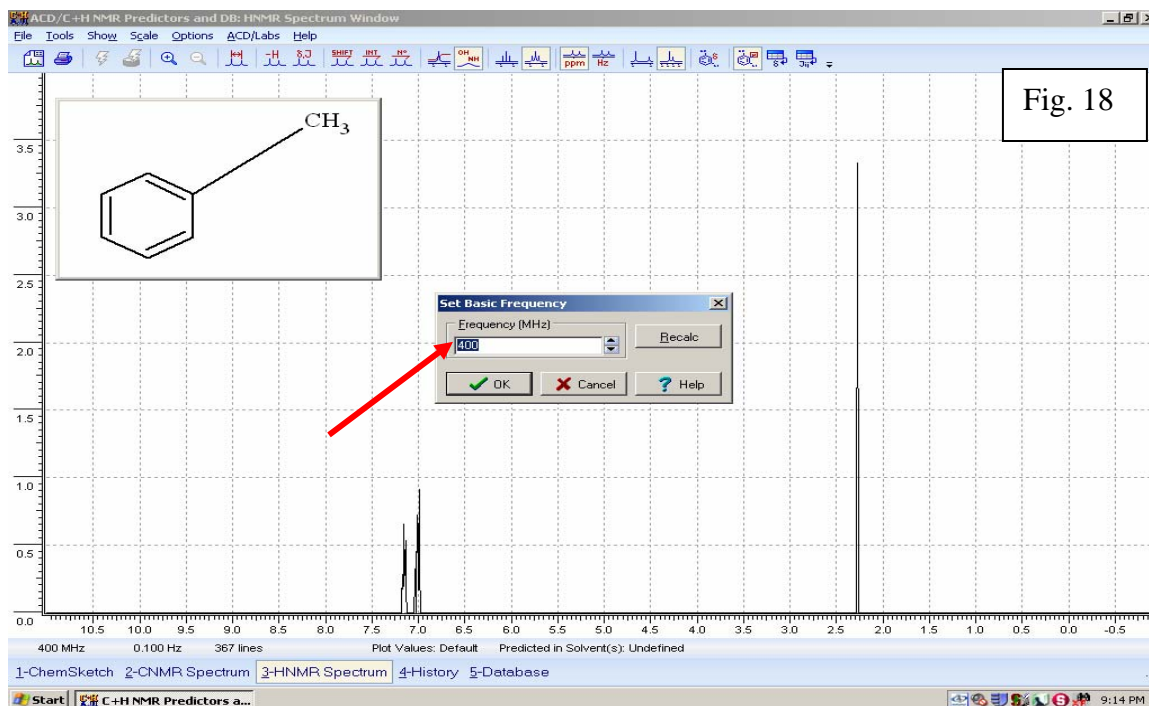
For example, you can left click on the icon at the green arrow shown in Fig. 16 to bring up a table of chemical shifts [orange arrow] vs their corresponding H positions [left side of table], and with an estimate of the uncertainty of each of their values [the column to the right of the column highlighted in green]. And you can left click on the icon at the red arrow, and bring up all of the ²J, ³J and ⁴J coupling constants. You can also select the same tables under “Show” from the top menu.

You will notice that the chemical shift for the H shown by placing the cursor where the blue arrow is on the ring in Fig. 16, is assigned a chemical shift of 7.00 ppm in the table [orange arrow in table]. Notice that this chemical shift is assigned to the midpoint of a group of peaks in the spectrum, and that once a given H is selected, the corresponding midpoint will be boxed in red in the chemical shifts table, and the corresponding relevant coupling constants will also be boxed in their table. Also we see from the chemical shifts table that this H has been assigned a position number on the ring of 6 [i.e., Group 6], and if you selected each of the other H's on the structure, you would find each of the other assigned positions. In this case if you go counterclockwise from 6, the values decrease until you reach the position that is symmetrical to 6, on the opposite side of the ring, and that would be position 2, ... and indeed their values for chemical shift can be seen to be identical.

Now let us change the default frequency of 400 MHz to a different value, and use it to recalculate the spectrum. Left click on “Options” [red arrow, Fig. 17], then left click on “Default Basic Frequency”.



This will bring up the screen in Fig. 18. Type in another frequency in place of the 400 [red arrow Fig. 18]. We will use 100 MHz for this example, then left click “OK”.



Then left click on “File” [red arrow, Fig. 19], and left click on “Recalculate Spectrum” just under “File”.

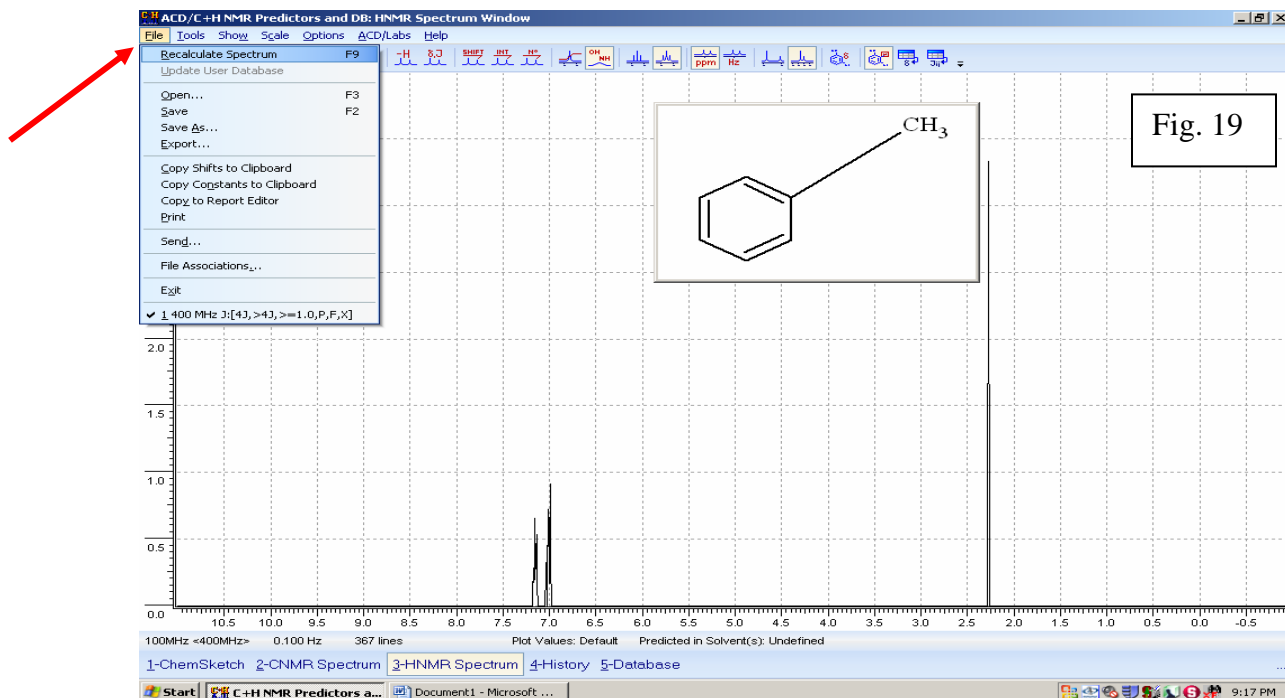


Fig. 19

This will give the screen shown in Fig. 20. Note the two peaks that were resolved at ~7.00 ppm in Fig. 19 are now no longer resolved, but instead are merged into one peak. Yet the midpoint of 7.00 remains the same. One could expand the scale as shown in Fig. 13, to see the two separate peaks, and their multiplicity.

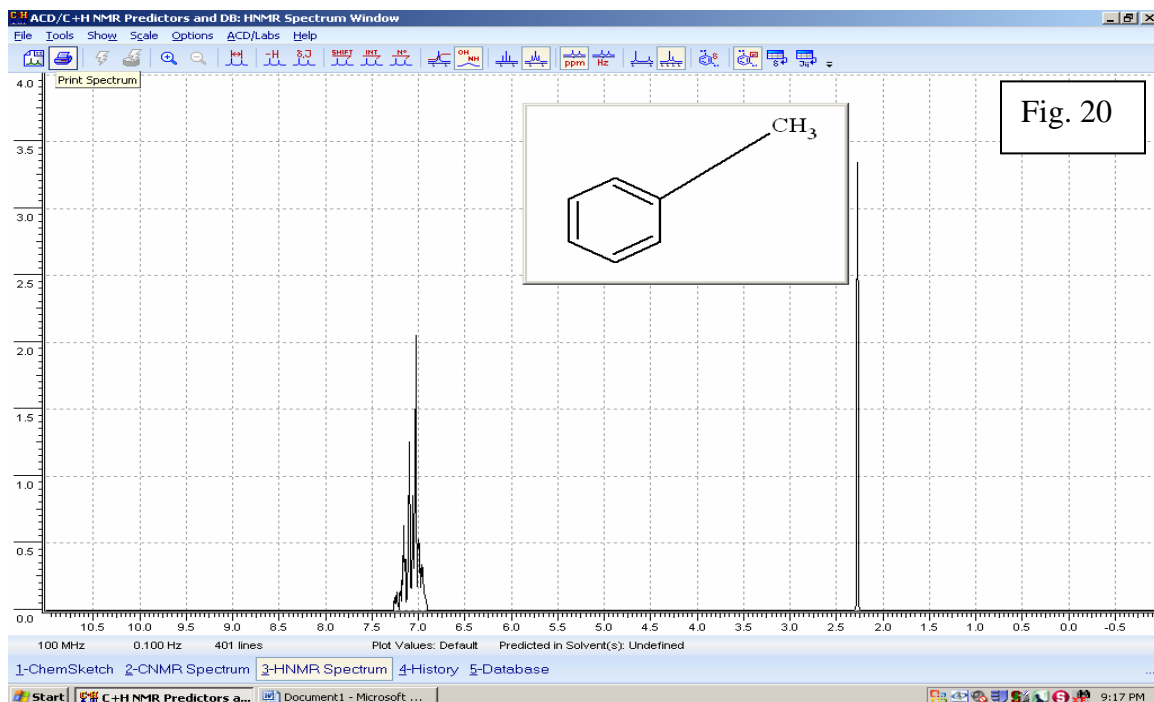


Fig. 20

One can also use ACD to predict the boiling point of a given compound. To do this for toluene, left click “1-ChemSketch” [red arrow, Fig. 21]. Then left click “Tools” [green arrow, Fig. 21]. Then left click “Calculate Boiling Point” [orange arrow, Fig. 21].

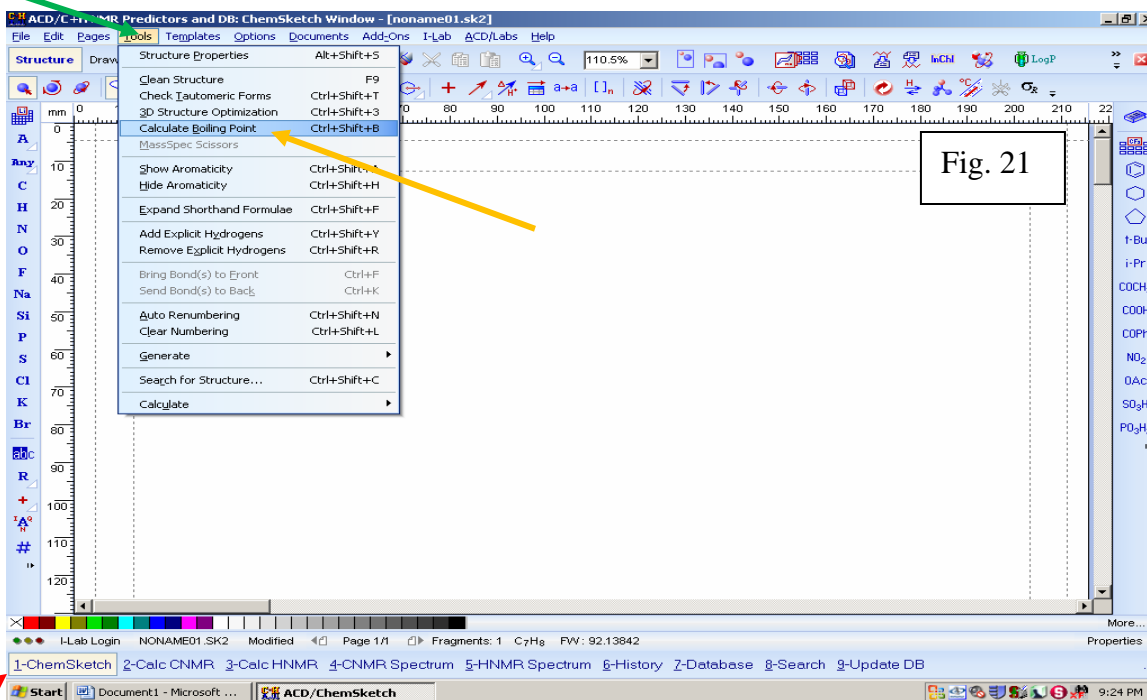


Fig. 21

This will show the boiling point both graphically and in tabular form to be 110.6 deg C, as shown in Fig. 22.

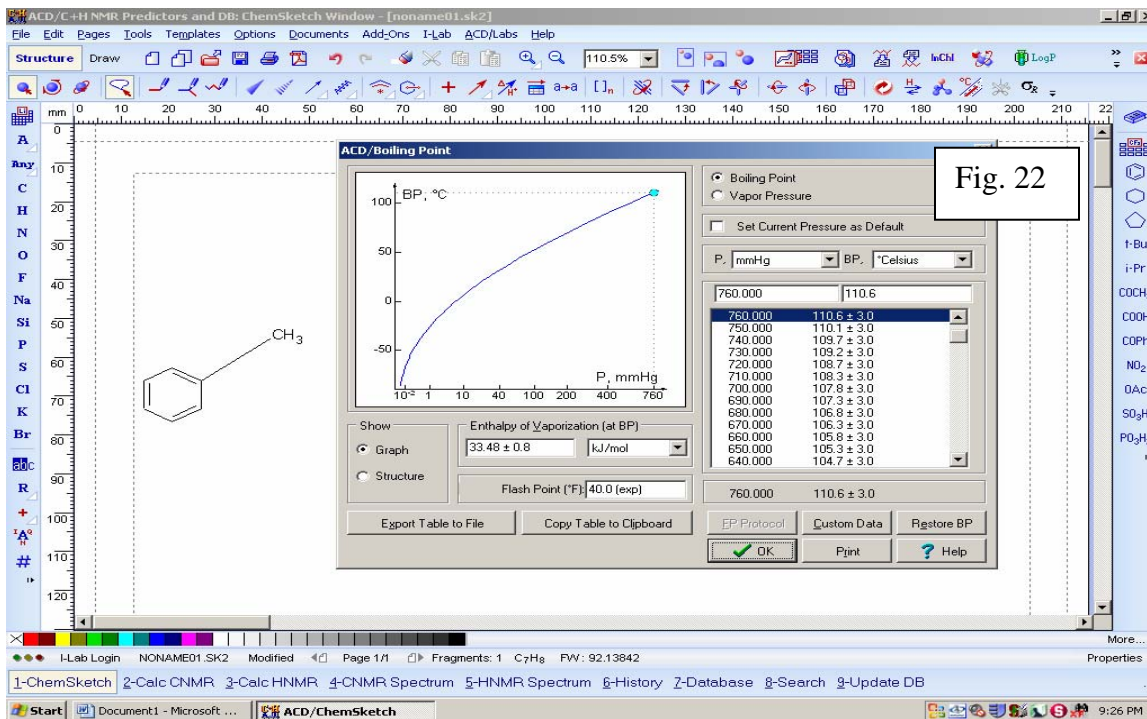
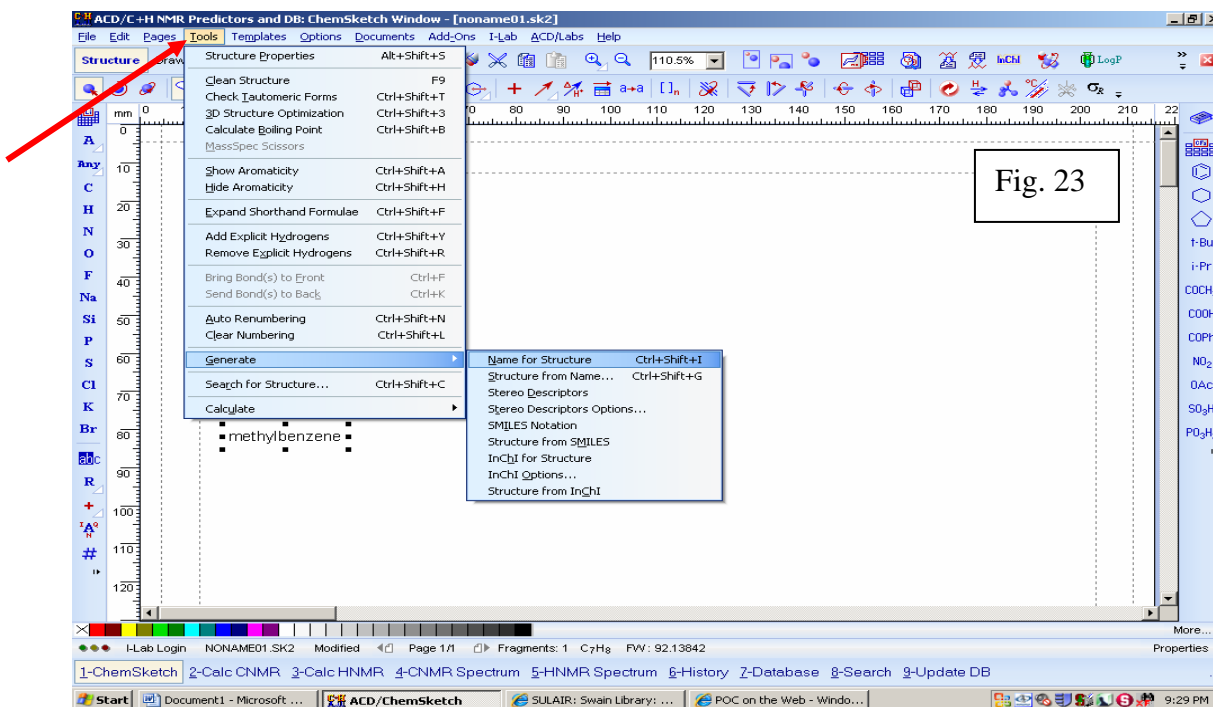


Fig. 22

One can also use ACD to generate an IUPAC name for a compound as well. Left click on “Tools” [red arrow, Fig. 23], left click on “Generate”, and left click on “Name for Structure”.



This will put the IUPAC Name in a box under the compound structure. Left click in the drawing area away from the box to remove the dots.

