


1. Open Mnova (icon on the desktop or the bottom horizontal strip), I placed a “view” of the Mnova screen at the end of this exercise.
2. Find the folder with your NMR spectra in it (I placed a “eugenol” folder in the documents folder for this exercise, everyone will use this folder)
3. Drag the eugenol folder into Mnova work area (a proton and a carbon NMR spectrum should open in the thumbnails on the left side too)
4. Click on “Save As” and save with both of your first names.
5. In the “thumbnail” pictures of the spectra on the left, right click on the top spectrum then click down below and copy the top spectrum, (I found that I could only use the “paste” function from the top pull down tabs), you should now have 2 copies of the top spectrum
6. Do the same for the second spectrum and paste it into the thumbnails, This will give you a working copies to modify and still keep the original spectra unchanged in case you need to use them again
7. Click in the working copy of the **carbon** spectrum in the thumbnails section (second carbon spectrum) to activate it in the main work area
8. You can use the mouse roller wheel to make the peaks in the spectrum bigger or smaller, (fit the largest carbon peak to less than half of the page)
9. To assign the solvent peak as a reference, click on the “expand” button (magnifying glass with plus sign, first button past the “entire page” pull down menu at the top in the button row), a magnifying glass with a plus will appear instead of the mouse arrow in the work area
10. Use the magnifying glass (plus sign in the middle marks the location) to mark the left side of the solvent region and drag it across the solvent to the right side and the spectrum will expand to those dimensions to show a large solvent triplet
11. If it is not what you want you can click on undo (control-Z) to go back to the previous display, also if you ever activate a button you don't want to use or are done with it, press “escape” to turn it off
12. To mark the solvent chemical shift, right click the mouse button and choose “peak picking”, you will have several options, to mark the deuteriochloroform solvent shift choose “peak by peak” and for the carbon reference peak, click on the middle peak, a dialog box will open and label it as 77.0 ppm, (later, for the proton spectrum, do the same but mark the chloroform “singlet” as 7.24 ppm)
13. If you ever have to go back to the “full” spectrum, click on the third button (row 1) past the “entire page” pull down menu at the top, click this button to get back to the “full” spectrum
14. When each spectrum is opened there is a “title” in the upper left corner that sometimes blocks peak chemical shifts, if you want, you can turn this off by right clicking the mouse and going down to the bottom of the list and click on “properties”, unclick the “title” box to turn this off (in the middle of the properties box)

15. Click on the “expand” button (magnifying glass with plus sign, first button past the “entire page” pull down menu), a magnifying glass with a plus will appear as the mouse symbol (as above)
16. Use the magnifying glass to mark the left side you want and drag it across the entire spectrum to the right side you want and the spectrum will expand to those dimensions (the full work area)
17. To mark your carbon chemical shifts, right click the mouse button and choose “peak picking”, you will have several options, if there are not too many peaks “manual” works well to label only the peaks you want, also, either “automatic” or “manual threshold” will work too (try them out if you want), if it’s not what you want, click on “undo”
18. If you have some carbon peaks that are really too close together to see, you can introduce an expansion of that region in the carbon spectrum, to practice this click on the sixth button past “full page” menu called “expansion”, (I call this an “inset”)
19. For practice let’s expand the carbon “solvent” peaks, as before drag the “mouse” magnifying glass across the region to be expanded and inserted into the full spectrum, a small box will pop up in the upper left corner with that region expanded, click inside that box to activate the box (green squares around the box), you can make the peaks larger or small with the roller wheel on the mouse
20. If there are peak values you do not want, you can right click on the mouse and go to “peak picking” and either click on “delete all” or “delete manually”, you can also do this with the integration later in the proton NMR
21. There is a green “anchor” button just above the expansion display that will allow you to move this anywhere on the screen you want if you left click on it and hold the mouse button down while you drag it around, if you plan another expansion it is best to move the first expansion away from the top left corner so they don’t display on top of one another.
22. Once you click inside the area of the display, the mouse wheel will size the display larger or smaller, as you wish, you can grab the right or left side of the box and expand or contract the size of the box, as you wish, you can also click on the expand spectrum button and spread out the peaks more inside the expansion box (inset display)
23. Click outside the expansion box (inset display) display and the full spectrum becomes active again
24. This completes our processing of the carbon 13 spectrum
25. Now click inside the “working” **proton** spectrum (the second one) in the thumbnails area on the left, this will add the proton spectrum to the work area
26. As above, expand the solvent region (7.24 ppm) and reference the chloroform peak at 7.24 ppm using a right click on the mouse (→ reference, → peak by peak)
27. If the “title” in the upper left corner gets in the way of chemical shifts, right click the mouse button, left click on properties at the bottom and unclick “title” in the properties box
28. To integrate, right click the mouse and choose “integration”, I like to use “manual” because I can exactly choose the regions I want to integrate, there is a little arrow head that points to where you want to start and finish the integral, curvy green vertical lines will show above and numbers will

appear below each of the chemical shift regions chosen, these represents areas under the peaks and show the relative ratios of the protons present

29. However, you can also use “autodetect” and let the program decide where to integrate and it will do the integration for you
30. In the “thumbnail” pictures of the spectra on the left, right click the mouse inside the box and choose “create new page”, we will use this blank page to copy in all of the expansions you make of the proton regions from the “working” proton spectrum
31. Just as you did to expand the carbon solvent peak, choose regions of the proton spectrum where the details are hard to see
32. Use the “expansion” button (6th button over from the “entire page” pull down menu) and drag across the desired region to be expanded (If you are using my eugenol example, choose the same 4 regions I expanded and process them one at a time onto the blank page)
33. Manipulate each expansion in a similar manner in my example page and then right click on the mouse and “cut” it out of the “working” spectrum,
34. Click inside the newly created page in “thumbnails and then click in the new page work area and paste the expansion into the new page, locate it in one of the corner areas because you will be adding 3 more (move the displays around with the top middle small “green” box)
35. Repeat this process for the other 3 “expansions” shown in the examples
36. You are now down with the proton exercise. There should be 5 spectra pages in the thumbnails: 2 original (H and C), a modified carbon NMR, a modified proton NMR and the proton expansions.
37. Print out pages 3-5 to turn in with both of your names written on the same spectra.
38. Do NOT save your changes in the “eugenol” folder. Remember at the start, you created a folder with both of your first names
39. Turn those pages in at the next lab period with both of your names on the spectra

Mnova screen

file edit view processing analysis advanced stack mass analysis predict scripts documents help																← pull down tabs												
1	2	3	4	5	6	7	8	9	10	11	entire page	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	← row 1 buttons
several possibilities, some of which are also controlled by right or left mouse clicks																← row 2 buttons												
V a r i o u s b u t t o n s			<p>1 = zoom out (expand button) 2 = zoom in (contract in steps until full spectrum) 3 = full spectrum 4 = manual zoom (type in left / right numbers in dialog box) 5 = pan 6 = expansion of a subregion as a separate display (I call this an "inset") 7 = fit vertical scale to most intense peak (all peaks) 8 = fit vertical scale to most intense compound peak (not solvent?) 9 = increase vertical scale (I use the mouse roller wheel) 10 = decrease vertical scale (I use the mouse roller wheel) 11 = crosshairs (can locate chemical shift values) 12 = restore 13 = edit blind region (not sure what this does) 14 = edit script (not sure what this does) 15 = various report tools (looks like some good operations but I have not explored these) 16 = stop script (not sure what this does)</p> <p style="text-align: center;">spectrum work area</p>																									
thumbnails																												