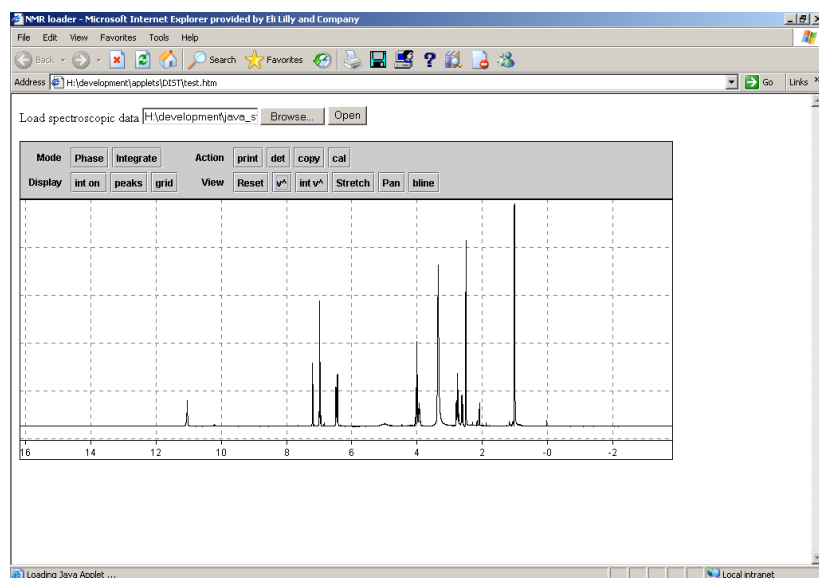# 1D and 2D NMR Viewers tutorial

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1D NMR viewer

When you open an NMR spectrum the applet should appear something like this:

(note that with the NMR viewers, you do not open your spectra from within the applet itself: you launch the applet from a web page by clicking on the sample of interest, or by selecting it a file in some other way from the web page: the applet has no 'file open' command.)

There are two parts to the NMR viewer – the spectrum itself and above it a control panel with a number of buttons which control the display.

Click on the spectrum with the mouse: a red line appears. Note that in the control panel at the top of the page, the chemical shift is displayed.
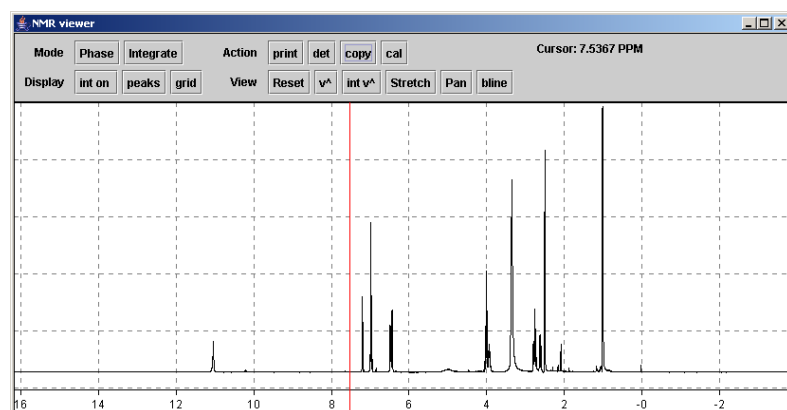
Press the mouse and drag it across the screen: a second red cursor line appears. The chemical shift and the difference to the first cursor is displayed in the control panel:
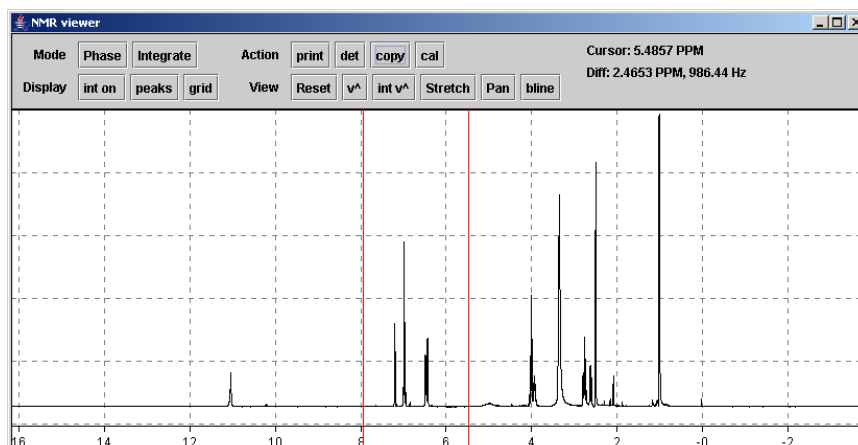

If you double click the spectrum now, the area between the red cursor lines is expanded. Zoom in closer on a peak in the same way. To zoom out again press the 'reset' button. Note that pressing reset once goes to the last zoom region: pressing twice zooms all the way out.
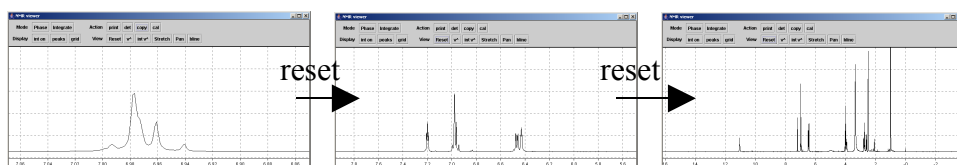
Try turning the mouse wheel to increase the vertical scale of the spectrum (ie how tall it is). You can also do this by pressing the 'v^' button, holding the mouse button down and dragging up or down.
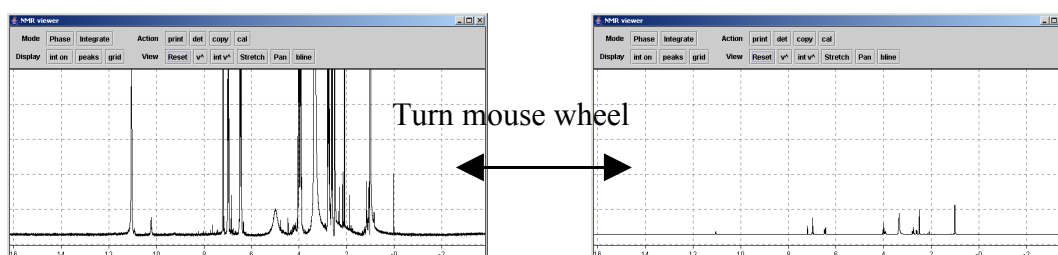
Try also clicking and dragging left and right with the 'pan' and 'stretch' buttons. These pan left and right across the spectrum, and stretch/shrink the spectrum horizontally. As well as dragging the mouse, you can hover the mouse over these buttons and turn the mouse wheel to have the same effect. This is particularly useful for panning – try it! This is actually a general feature: most of the buttons that operate by click and drag also operate in this way, ie you can hover the mouse over them and turn the wheel to get the same effect.
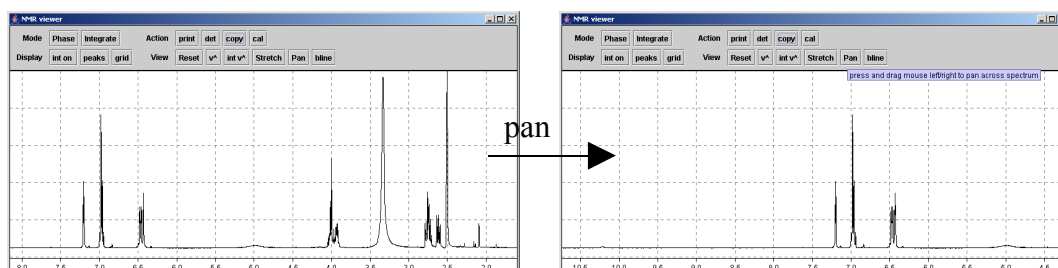

Try pressing the 'det' button the applet moves into a separate resizeable window. When you close the window, it goes back into the web page.

Notice also some of functions of the control buttons are also reproduced in the right click pop-up menu. Some other functions can only be accessed this way: they are described later on.

Phasing

Press the button in the top left of the control panel marked 'phase'. The screen should now look something like this. Note that the 'action' buttons change to those you need to do phasing. The PHC0 and PHC1 buttons adjust the zero and first order phase respectively: The PHC0 button affects the phase of all of the peaks in the spectrum equally, whereas the PHC1 button has an increasingly large effect the further away you move form the 'pivot point', which by default is the biggest peak in the spectrum.
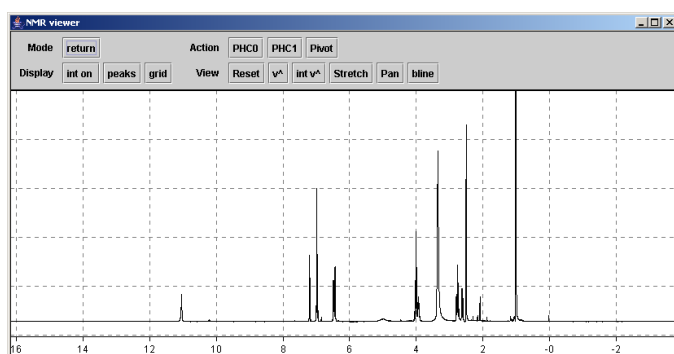
Using the mouse, press on the button marked 'PHC0' in the 'action' part of the control panel. Hold the mouse down and drag it up or down. The zero order phase of the spectrum changes. Do this until the largest peak is phased. Use the mouse wheel to make the spectrum taller – it is easier to see if the peaks are phased this way.
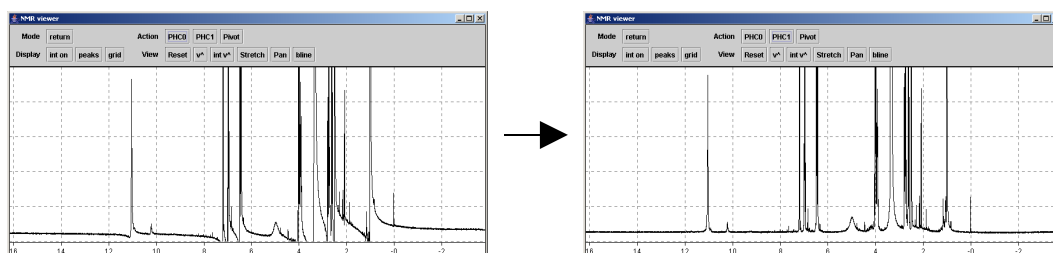
Next click on the 'PHC1' button and drag the mouse: this adjusts the 1st order phase. Drag the mouse until the peaks at the left and right extremes of the spectrum are also phased.
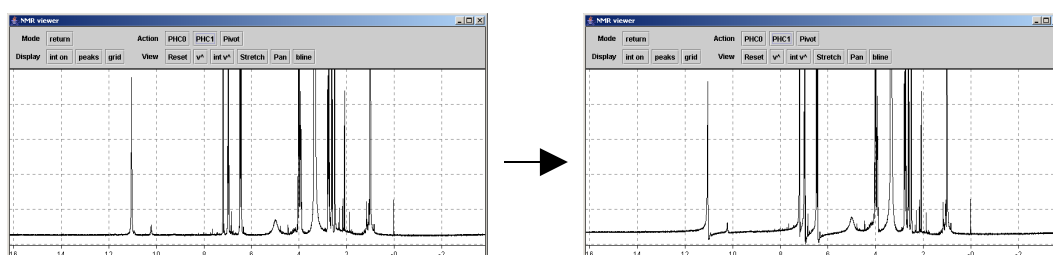
You can also move the pivot point (ie where the first order phase has no effect) if you want to. Click the pivot button – a red line appears. Click again to select the point you want to be the pivot. This usually isn't necessary, but can sometimes be useful.

You can also hover over the phc0 and phc1 buttons and turn the mouse wheel: this is useful to change phase quickly.

When you are happy with the phasing, click the 'return' button to finish.

NB if no imaginary data is available, the phase button will be disabled.

Calibrating the chemical shift

If the chemical shift scale on the spectrum is not correct, it can be referenced easily. Zoom in on the peak to be referenced to help locate it precisely:
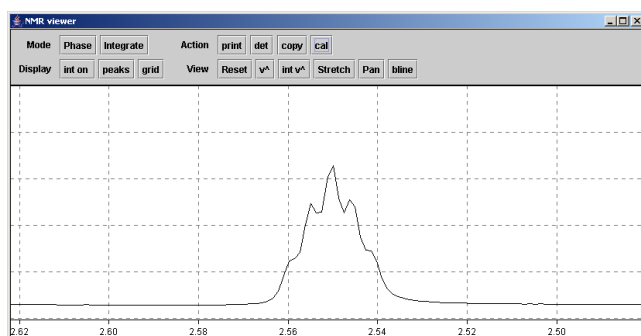
Click on the 'cal' button. A red cursor appears. Carefully align this with the top of the peak you want to reference and then click the mouse. A dialogue box will appear, asking you to enter the chemical shift value. Enter the value you want.. The shift scale changes to reflect the value you entered.
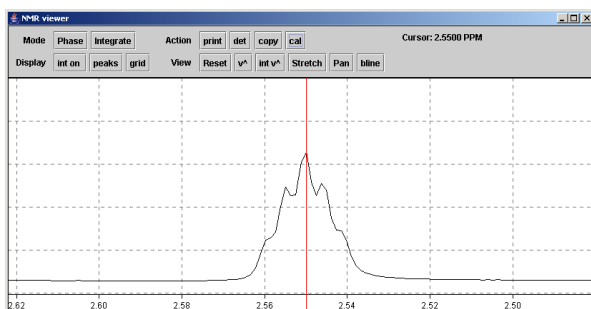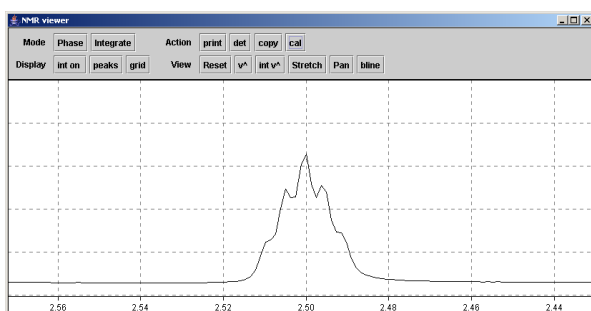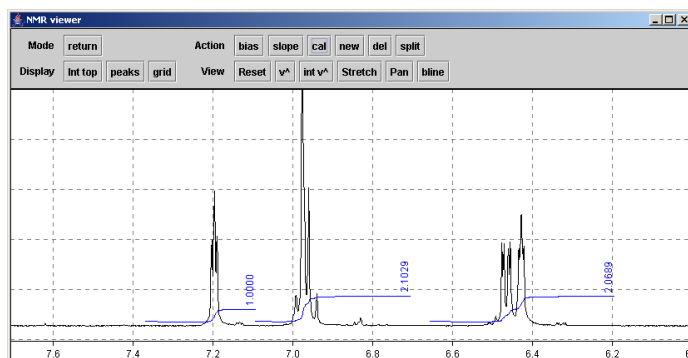
Integration

Click on the 'integrate' button at the top left: the action buttons now change to those needed for integration. The screen should look like this:

For Bruker data, the automatic integrals created by the NMR spectrometer are displayed if present. If you click on an integral, you can select it (it turns red). If you press the 'del' button, this integral is deleted. If nothing is selected and you press 'del' all are deleted. You will be warned before this happens!
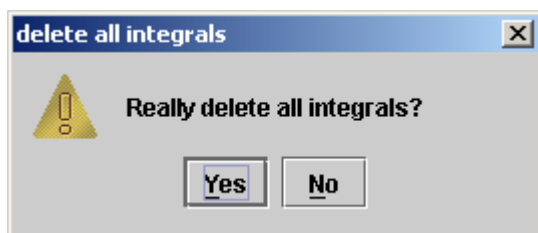
To define new integrals, click on the spectrum: move the cursor to the left of a peak, then press the mouse and drag as though you are going to expand. Press the 'new' button to define the area as an integral (you can also right click and choose 'new integral' from the popup menu).
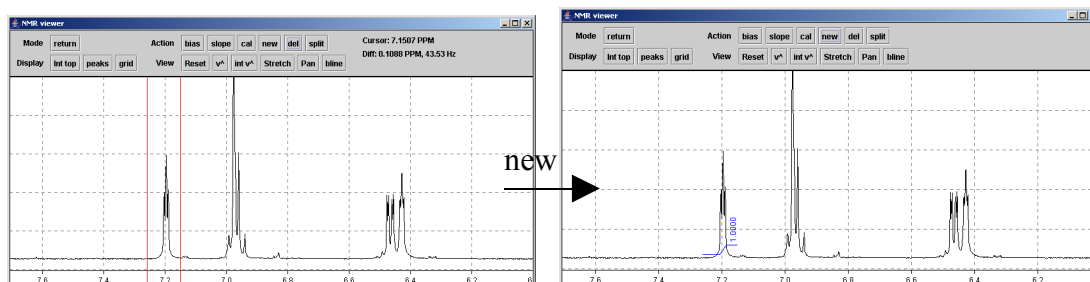
Click to select the integral: it turns red. Click the 'bias' button and, while holding down the mouse, drag up and down. Try the same with the slope button. Between them these two buttons can be used to make the region either side of the integral flat: bias affects the whole integral, slope the right more than the left (cf. zero and first order phase correction).[1]
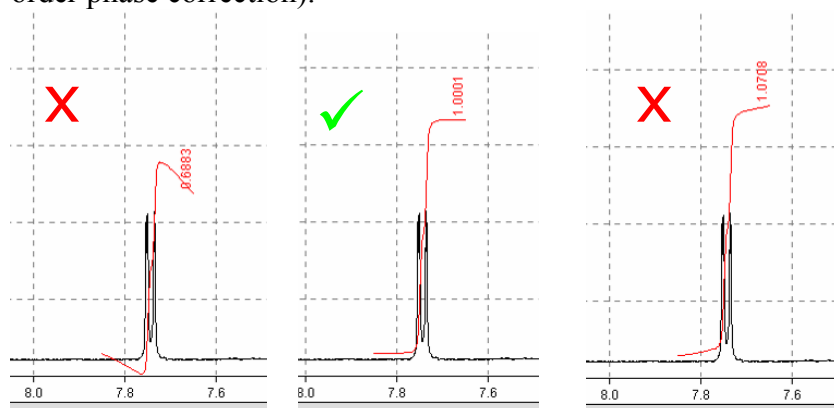

You can calibrate an integral to any value. click on the 'cal' button – a red cursor appears. Click within the limits of the integral. You will then be prompted for the integral value. Enter a number and press return – it is set to this value and all of the other integrals are calibrated relative to this.
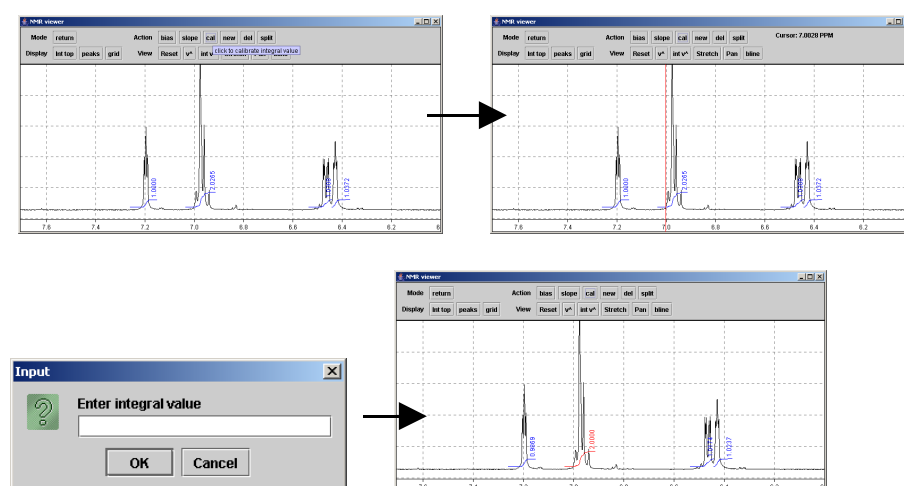
Try clicking and dragging on the 'int v^' button – this changes the vertical scale of the integral. You can also do this by holding down the 'shift' key on your keyboard and turning the mouse wheel. Try also holding down 'control' and turning the mouse wheel – this changes integral and spectrum scaling together.

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[1] What you are actually doing when you change the slope and bias is a baseline correction on the integral. The slope and bias are automatically corrected when you define an integral, so most of the time you won't need to change them.

You can also try splitting an integral – click split then click within an existing integral region. It is split into two.
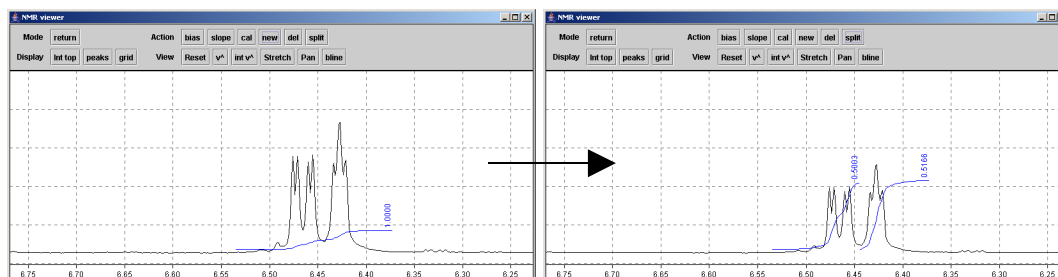

If you prefer, you can display just the integral values under the integrals. Press 'int top' which toggles the integral display modes: the integral now appears at the bottom of the peaks. Pressing again turns them off, once more goes back to the normal integral view.
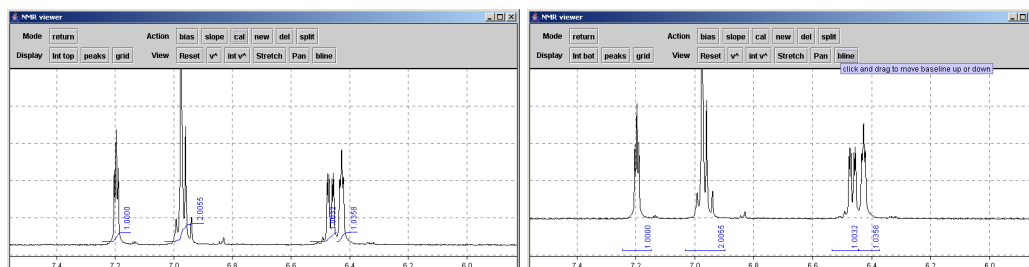

When you are happy everything is integrated OK, press the return button to leave the integral mode. You can also do this by right clicking on the spectrum and selecting return.

Peak picking

Click on 'peaks' on the 'display' part of the control panel. Peak picking is turned on. Try adjusting the vertical scale of the spectrum with the mouse wheel – make the spectrum taller and shorter. Note how the threshold for peak picking is controlled by how tall the spectrum is. Clicking the 'peaks' button once more puts the peak picking in Hz – useful for determining coupling constants. Clicking again turns it off.
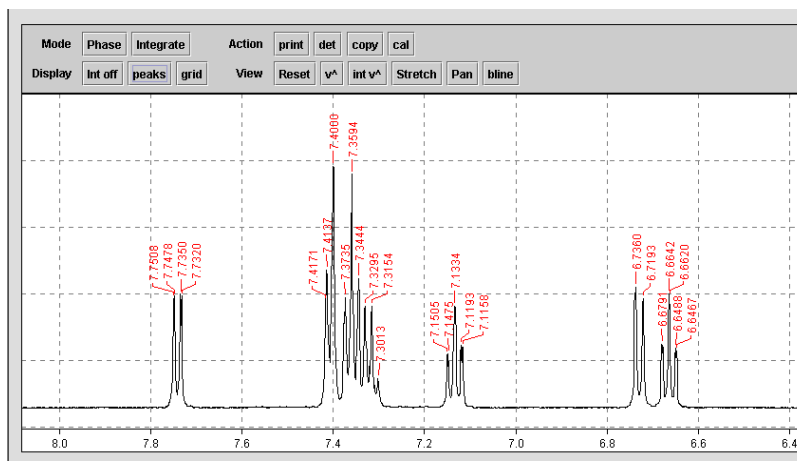
Note that if you hover the mouse over any of the buttons on the control panel, a 'tool tip' explains what it does:
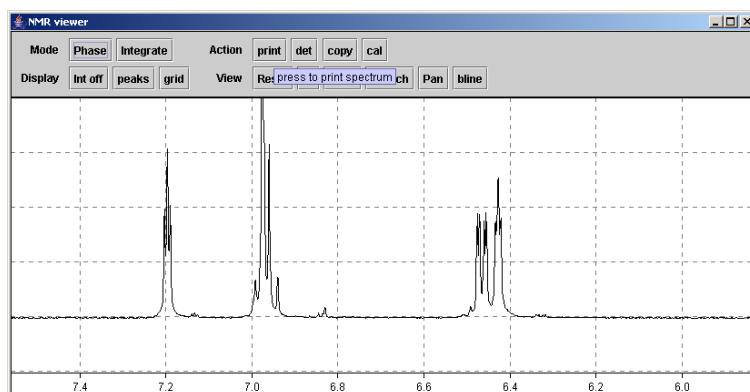

Printing

Printing is 'what you see is what you get'. The print out will appear exactly as the plot on screen – So if you want integrals or peak picking you have to turn them on. The buttons next to 'Display' on the control panel toggle these on and off. When you click print, a standard print dialog is displayed. Make sure to press the applet print button, not that in internet explorer.

Copy functions

Try right clicking on the spectrum – a list of options appears. One of these is 'copy spectrum'. This places a picture of the spectrum on the clipboard so you can paste into word, powerpoint, excel, etc. If you choose 'copy integrals', the integral values together with their start/end chemical shifts are copied. 'copy peaks' copies a list of the peak chemical shifts as displayed in peak picking. Note the latter two only work if the spectrum has some integrals or peak picking is on!
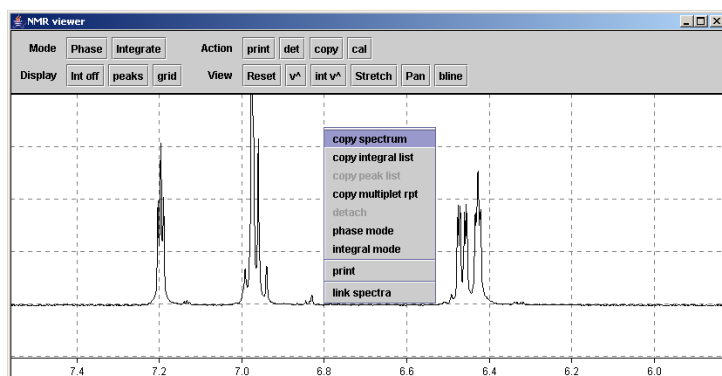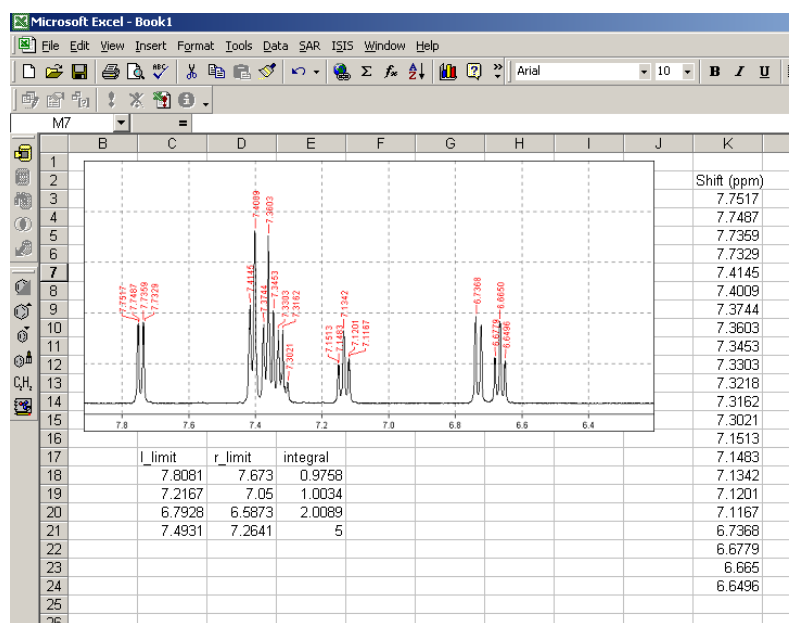
Multiplet report

A very useful feature is the multiplet report: to create it, right click and select 'copy multiplet rpt'. The multiplet algorithm works by trying to assign a multiplet type to each integral region you have created. In other words, you can help it do well by integrating each multiplet carefully. Assuming you have integrated the spectrum to give an integral to each 'multiplet' as you see it, this will attempt to analyse the multiplets and report them in journal/patent format. If it can't assign a multiplet type, it defaults to 'm'. The results are placed on the clipboard, and you can paste the results into word, powerpoint, etc. Eg:

1H NMR (500.13 MHz, MeOD): 7.74 (dd, J= 1.50, 7.91 Hz, 1H), 7.42-7.33 (m, 5H), 7.15-7.12 (m, 1H), 6.74-6.72 (m, 1H), 6.66 (td, J= 7.59, 1.07 Hz, 1H).
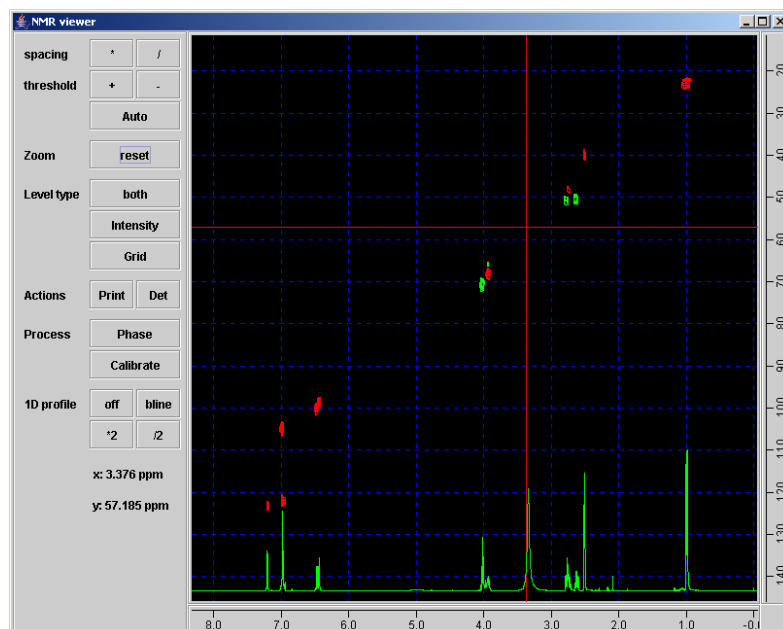
2D NMR viewer.

When the 2D applet is launched, you are presented with a view something like this:
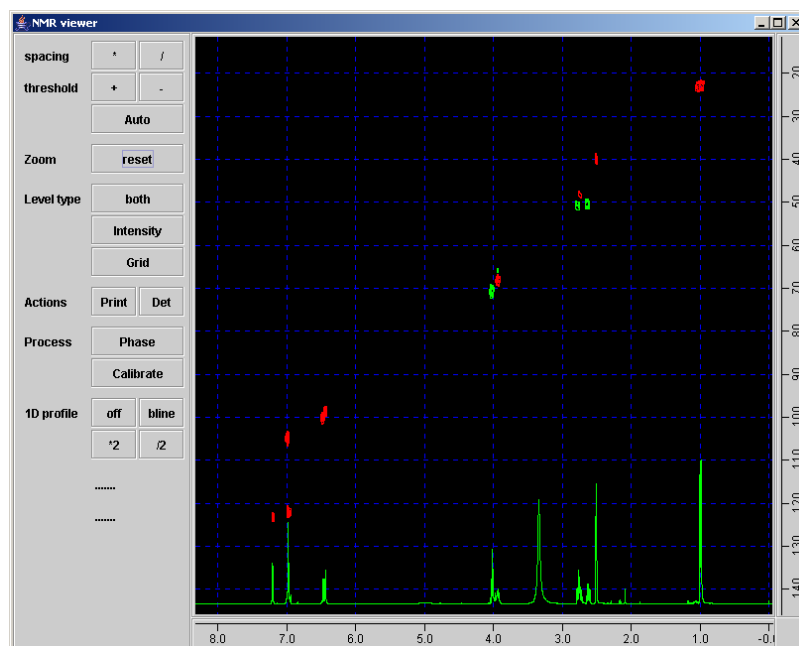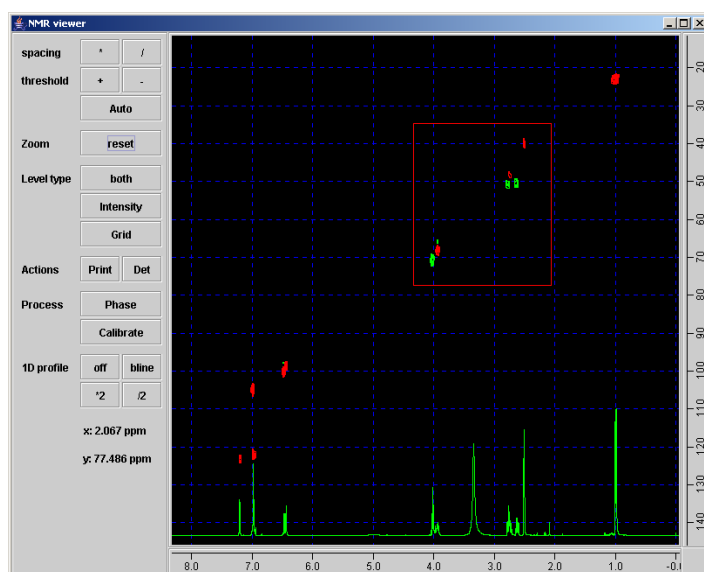

As with the 1D viewer, there are 2 parts to the display: the spectrum on the right and a control panel on the left.
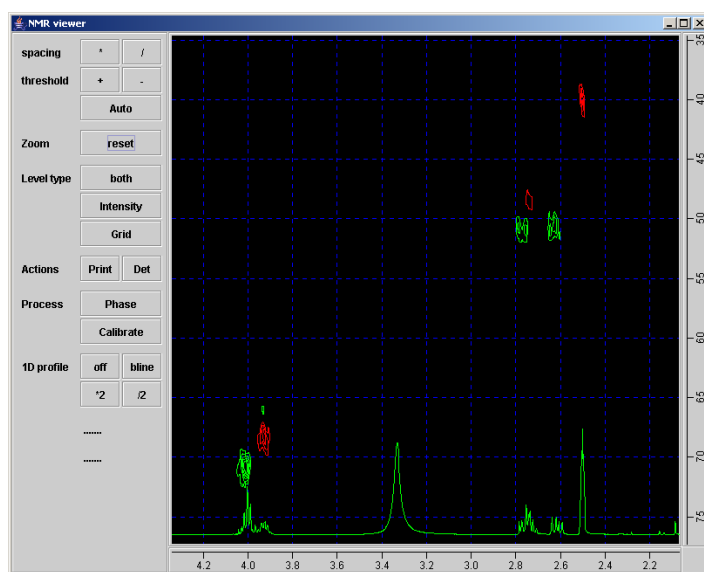
With the mouse, click on the spectrum. A red cross hair appears. The chemical shifts of the cross hair position appear on the control panel on the left.

Press the mouse and drag – a red rectangle appears as you drag it.

When the rectangle covers the area as shown above, let go of the mouse button, then double click the spectrum: you zoom in to the selected area.


The reset button works as for the 1D viewer: clicking once zooms out to the previous view, twice zooms to the full spectrum.

Using the spacing '*' or '/' buttons, try altering the contour levels of the 2D plot. You can also do this by turning the mouse wheel – this is the most convenient way to change contour levels.

The threshold buttons also affects the contour levels: try changing these too. You can also do this by pressing the 'shift' key on your keyboard and turning the mouse wheel.

The 'Auto' button resets them to their original values.

The spacing and threshold buttons actually control the position at which the contour levels are drawn. The spacing moves the top contour level and all the others proportionately. The threshold button moves the bottom contour level but leaves the top unchanged:
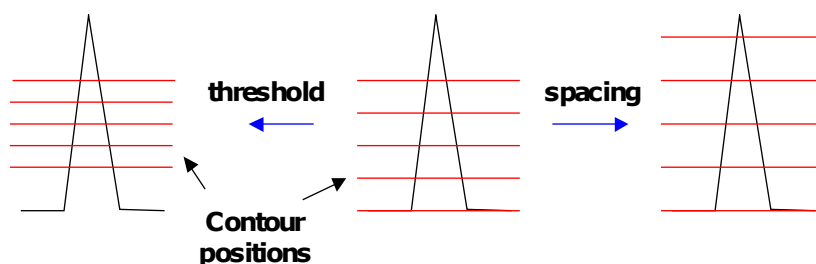

In practice spacing is usually enough, and this is conveniently controlled with the mouse wheel.

The 'on/off' button next to '1D profile' toggles the display of the associated proton spectrum (if available). Click the '*2' and '/2' buttons to change the vertical scale of the 1D profile: you can also do this by pressing 'control' on your keyboard while turning the mouse wheel. You can move the 1D profile up and down by pressing the 'bline' button and dragging the mouse up and down.
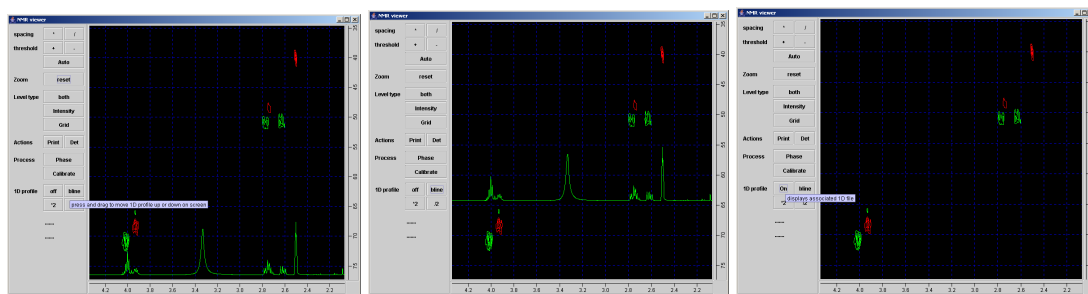

Now try clicking on the 'contours' button – this toggles between the display of contours lines (looks good but a bit slower to draw) and intensity levels. Contours look particular good when zoomed in – try zooming in on some of the cross peaks. The default setting is contours, but change to intensity if you want to speed up the program.
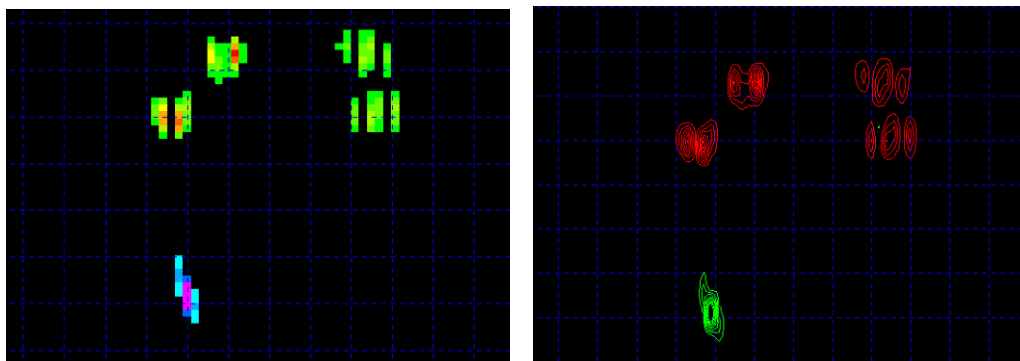
Click the 'level type' button toggles the display of contour levels between positive, negative and both. Try cycling through all three display types.
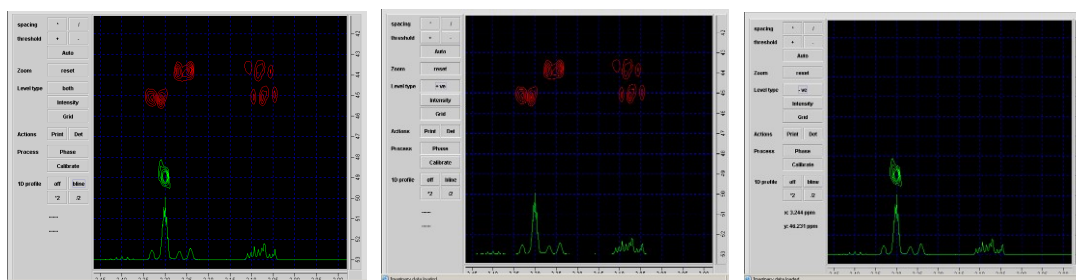
A number of commands can also be accessed by right clicking on the spectrum. One particularly useful one is 'copy spectrum' which places the currently displayed region on the clipboard, so you can past it into word or powerpoint.
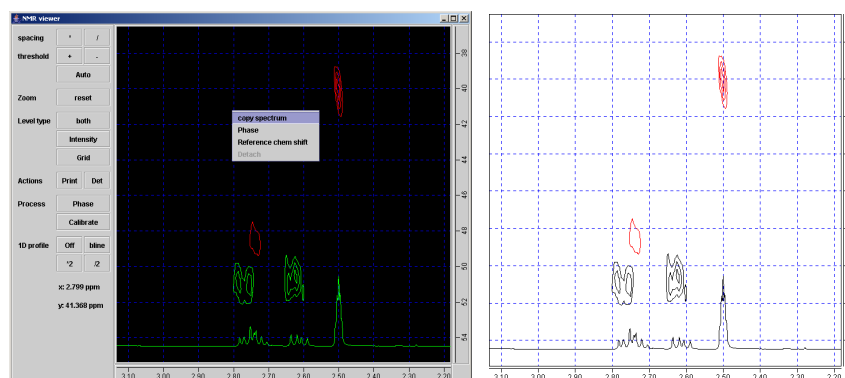

Try also turning the grid on and off with the grid button. The 'Det' button detaches the spectrum into a separate resizeable window – this allows you to make the 2D display as big as your screen will allow.
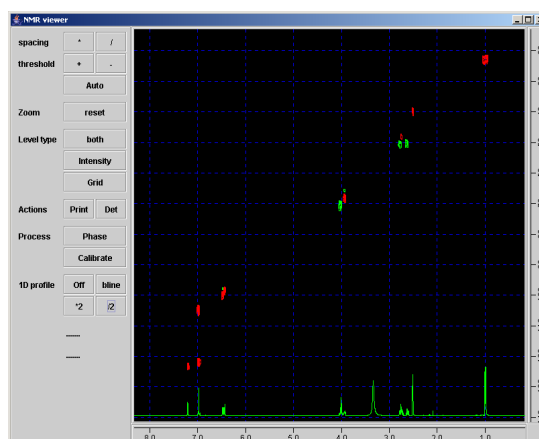
Phasing

To phase a 2D NMR we proceed by extracting two rows containing peaks at the left and right of the spectrum – these rows thus usually come from the bottom and top of the 2D respectively. The two rows are added together and then phased as for a 1D with zero and first order phase correction (see earlier 1D section). Finally the phase correction is applied to the whole spectrum.

To do this click on the 'phase' button. You will be prompted to select two rows, which you do by clicking on them with the red crosshair. After you have selected the second row, the 'imaginary' data required for phasing will be read in. This may take a couple of seconds. Once loaded, the sum of the rows will be displayed. Use the 'bline' button to move it to the centre of the display if necessary.
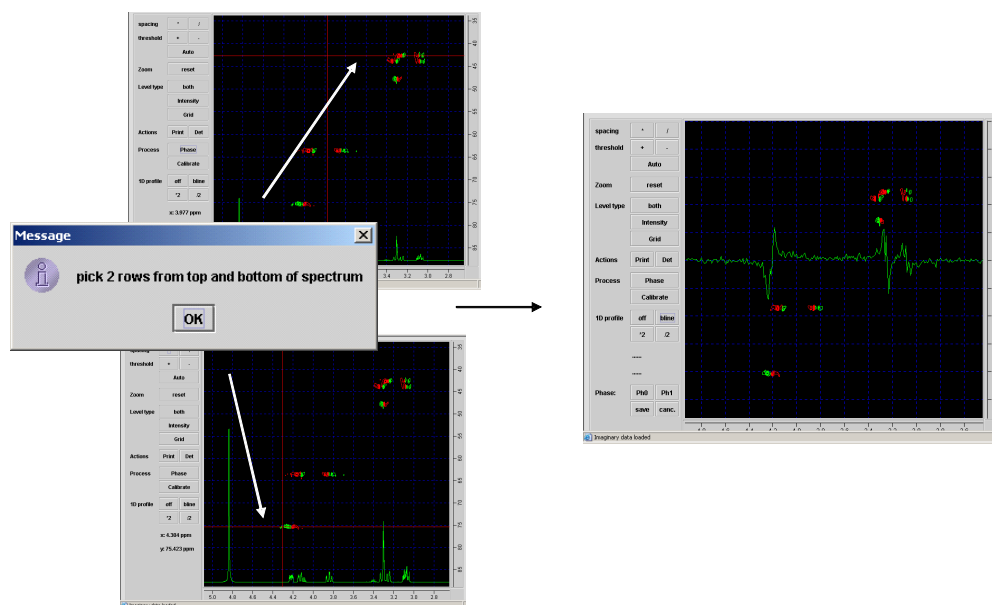

Note also that some extra buttons have appeared on the control panel under the heading 'phase'. Phase the spectrum by pressing the 'Ph0' and 'Ph1' buttons and dragging the mouse, as described for 1D spectra. Of course, in some 2D spectra, some of the peaks will have to be phased down rather than up – moving the profile to the middle of the screen with the 'bline' button is helpful here.[2] Click save when you are happy all is OK.

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[2] Some 2D spectra (eg most HMBC and many COSY experiments) are so called 'magnitude' processed. They do not need to be phased and indeed cannot be phased. If you try to, you will get a message saying it is not possible. Magnitude spectra are not as sharp, however, as 'phase sensitive' ones, which is why it is worth going to the trouble of phasing when possible.

Referencing chemical shift

Next, we will calibrate or reference the chemical shift scales. Zoom in on the region around a reference peak. Click on the 'calibrate' button. The red crosshairs appear. Carefully click on the centre of the peak. A dialogue box appears: enter the f2(x) shift. Choose to apply this just to the 1D, 2D or both as appropriate. Next enter the f1(y) shift. The spectrum is updated to reflect the new values.
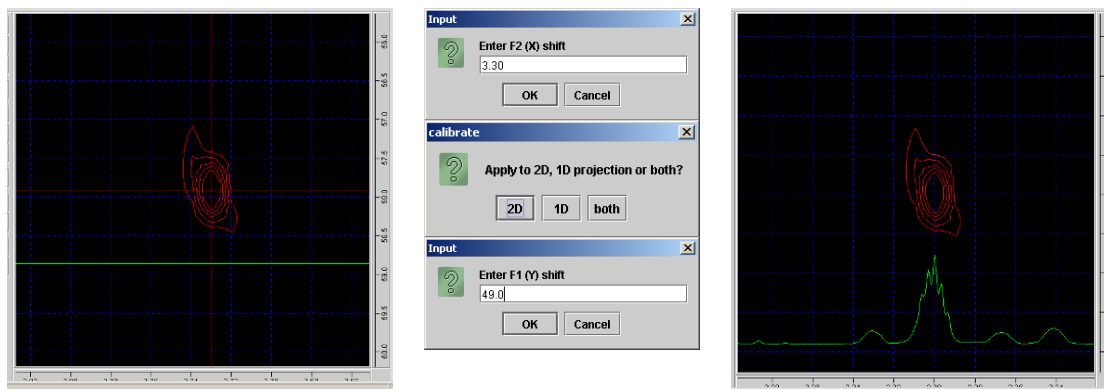
Printing

When you are happy with the display, click the 'print' button. A normal windows print dialog is displayed which lets you choose your printer. If you click OK, a page dialog comes up so you can change paper if you want (eg to A3 for a big plot).
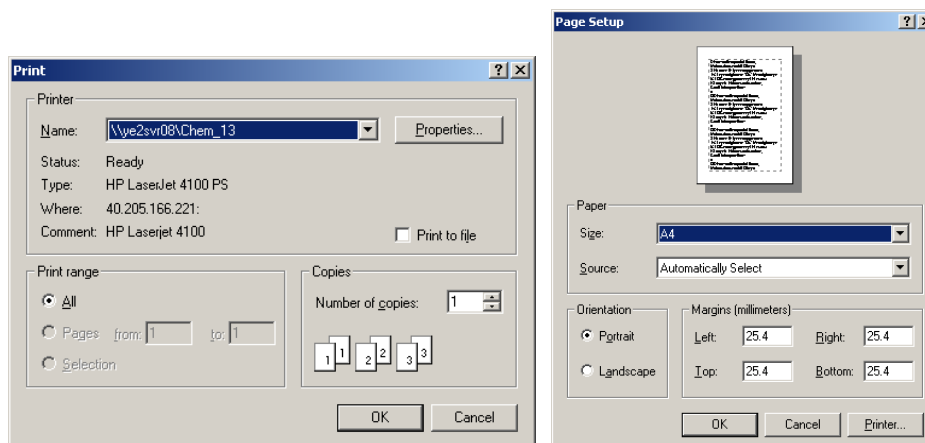
The print out you get should reflect exactly what you see on screen: the zoom region will be as is displayed, if you have the profile or grid turned on, they will be printed. The print-out also contains sample title and other useful information.