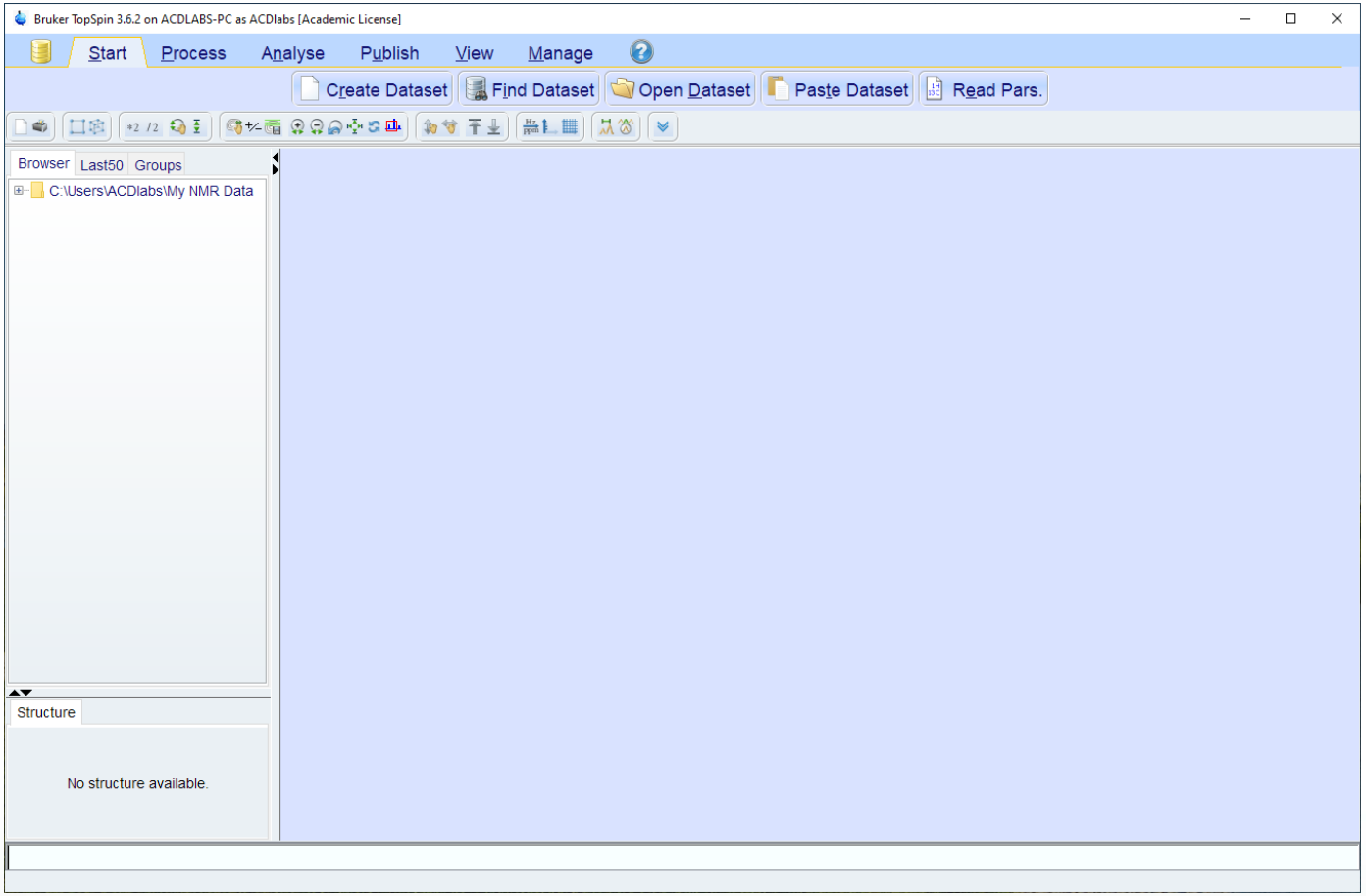
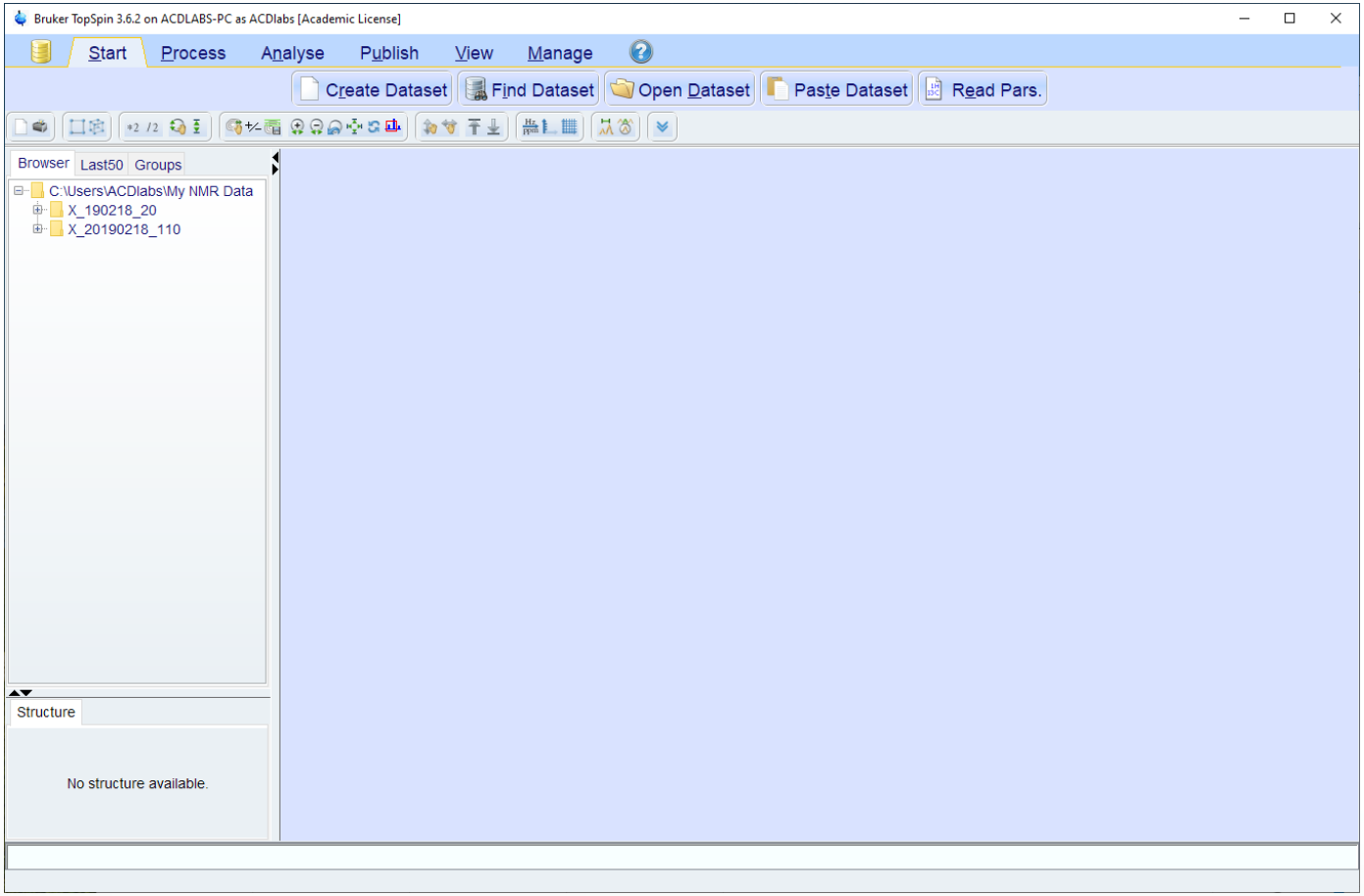
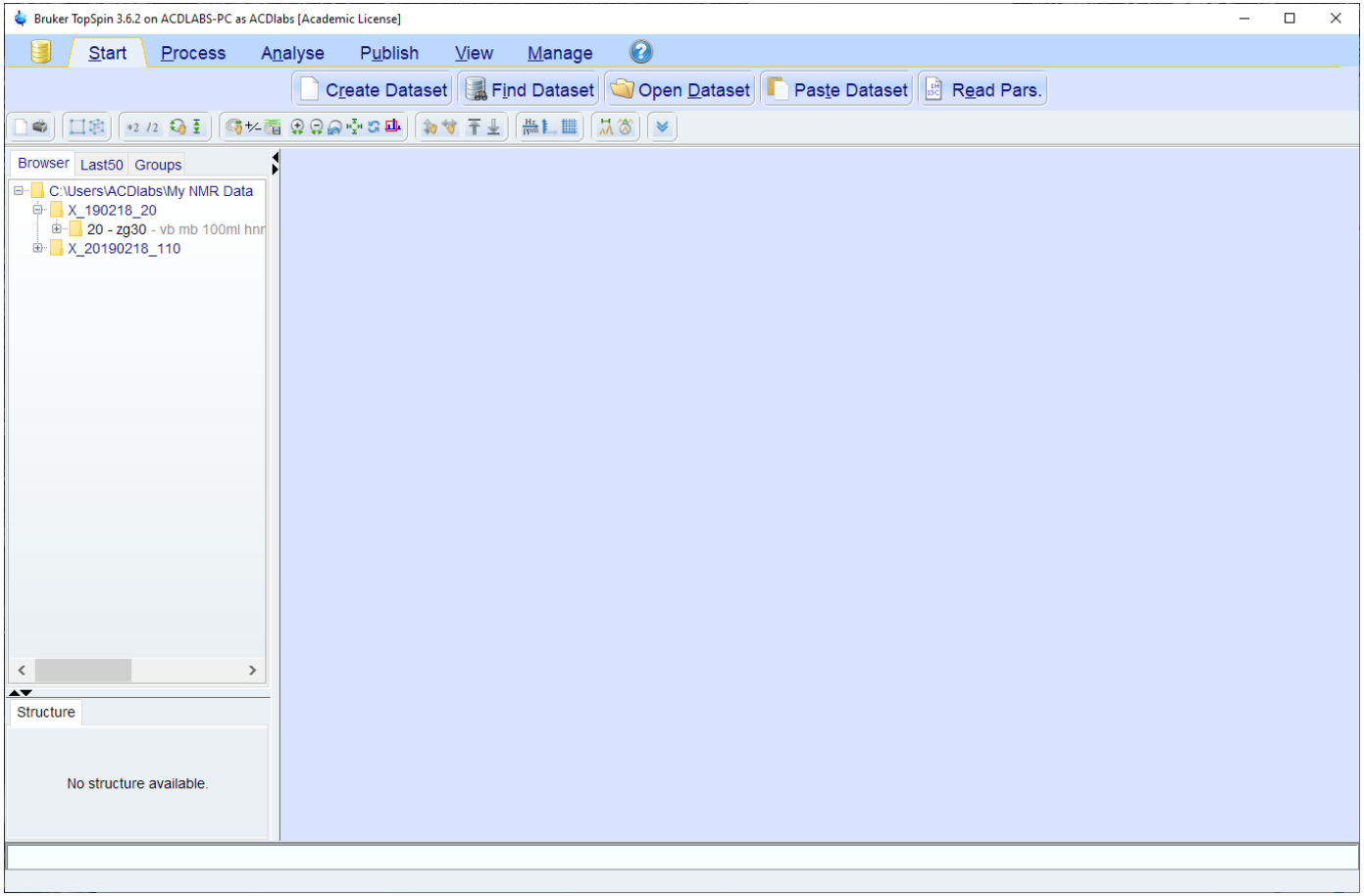


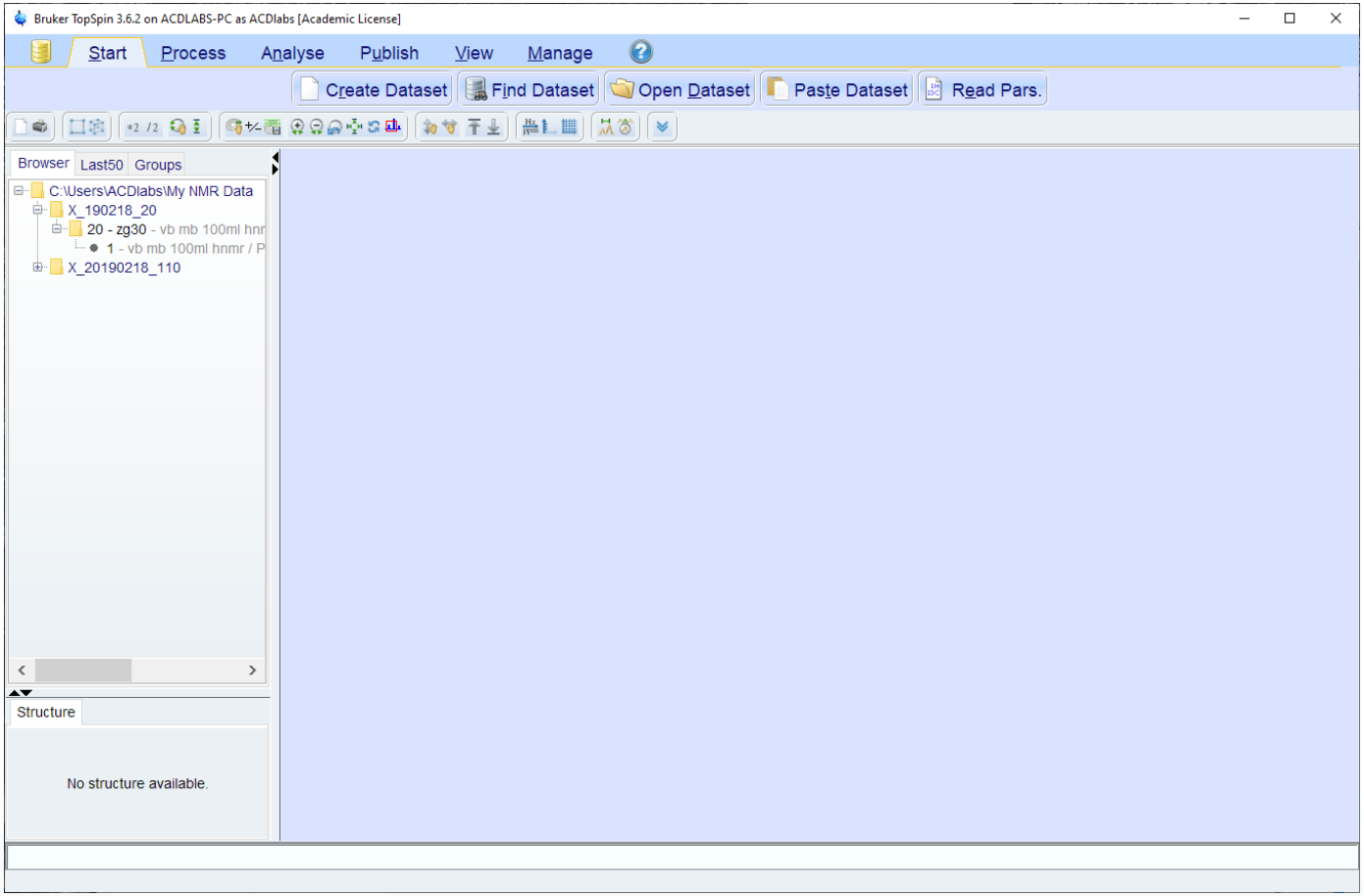
When you open TopSpin it usually looks something like this… there is no dataset open yet.



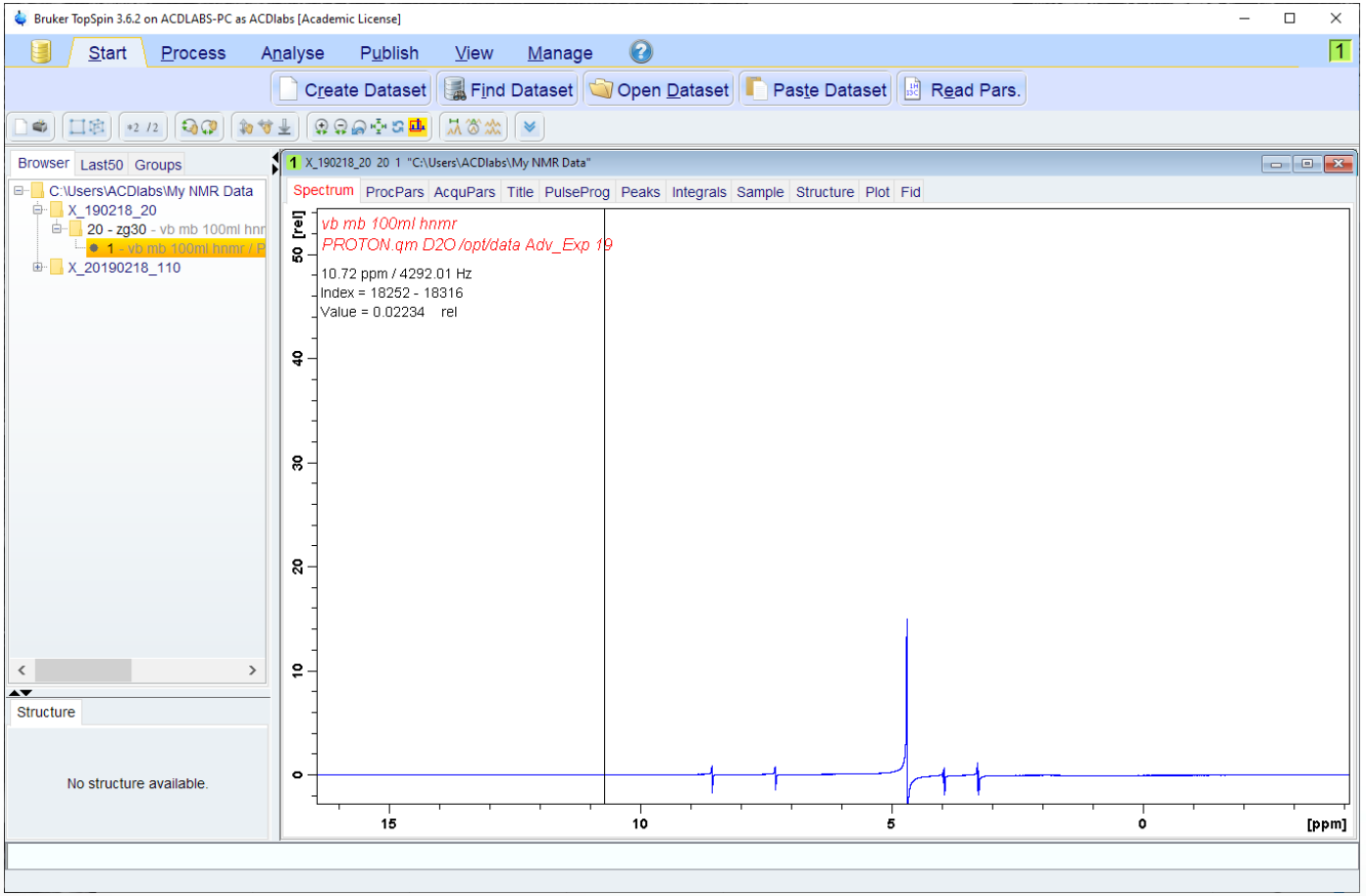
When you click on the “+” next to the folders in the browser pane it will expand to the next level.



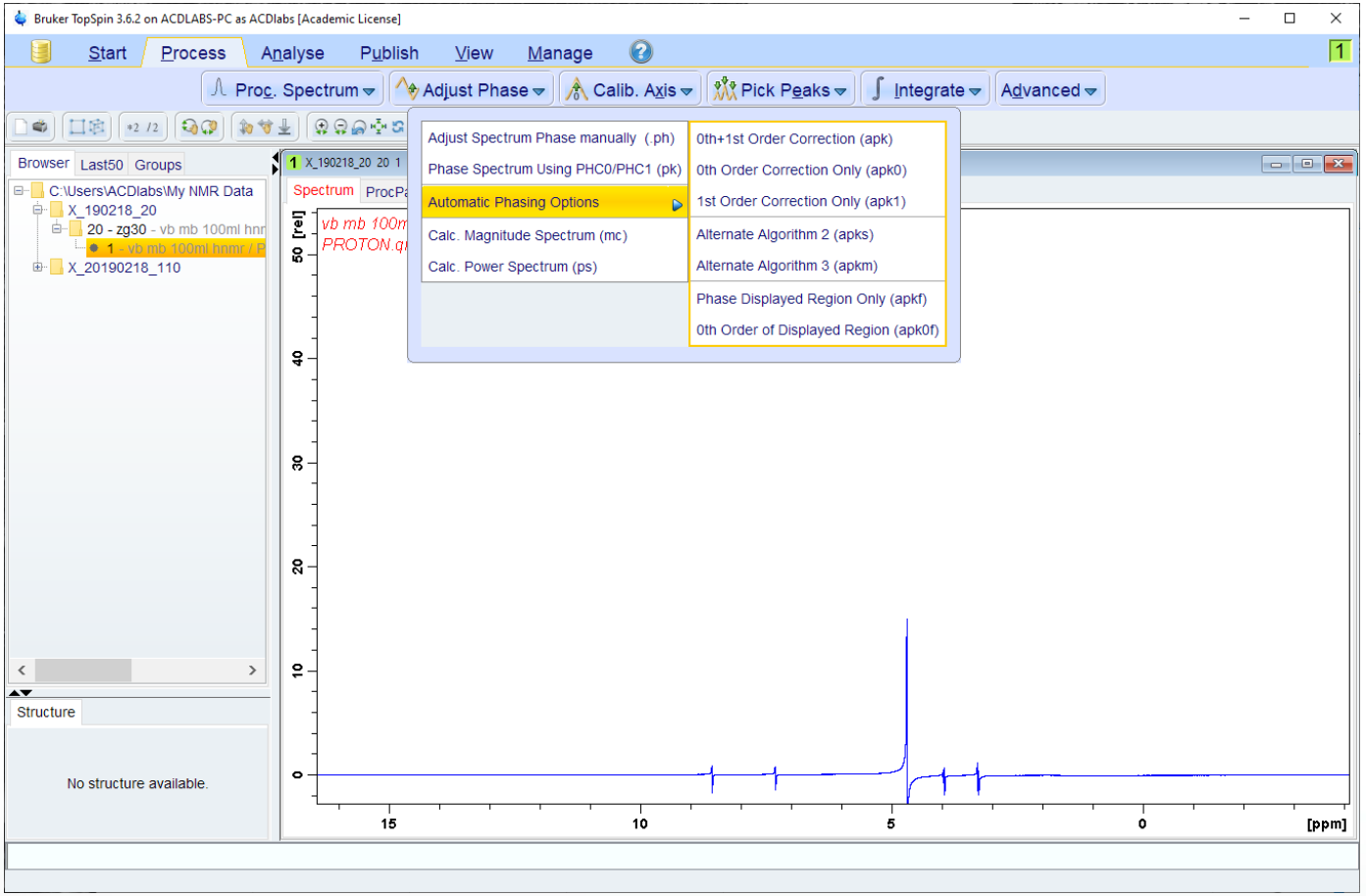
The first level is the experiment name, the next level is the experiment number (here, 20).



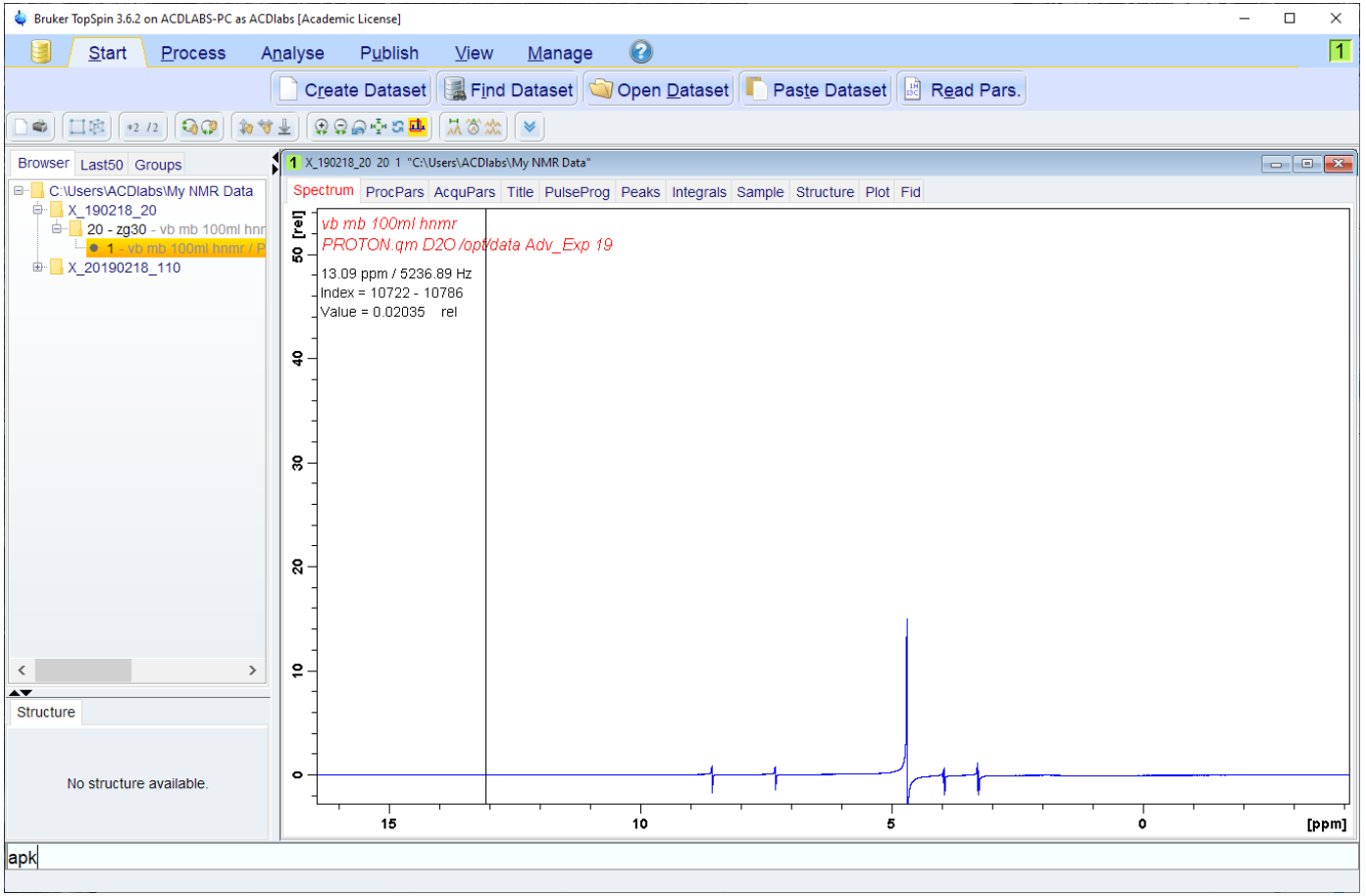
The bottom level (usually a “1”) is the processed data for the experiment – double-click on it and the spectrum will be displayed.



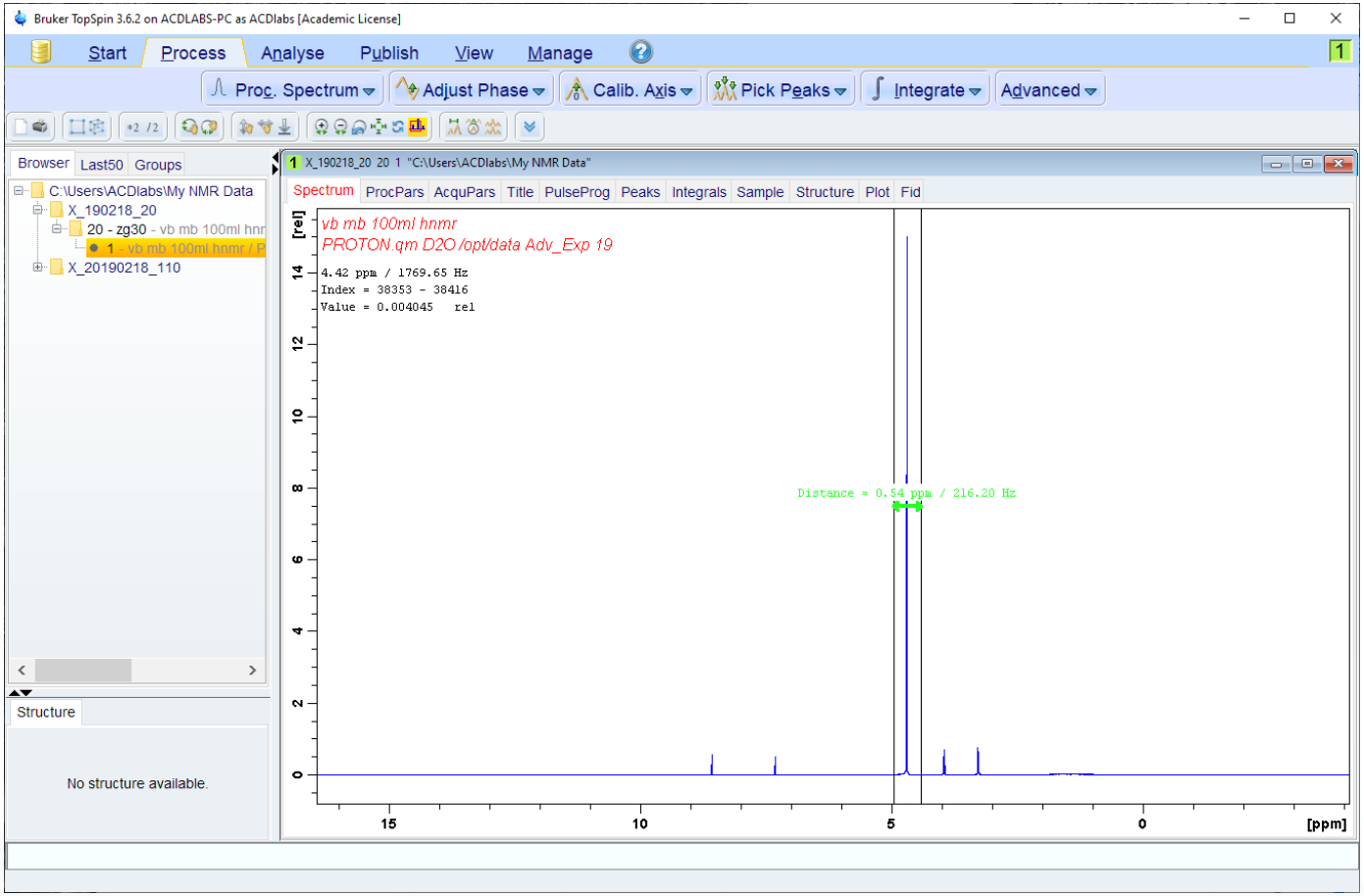
Often, when you open it the data will look like this… the lines are out of phase. They should be absorptive, these are dispersive.



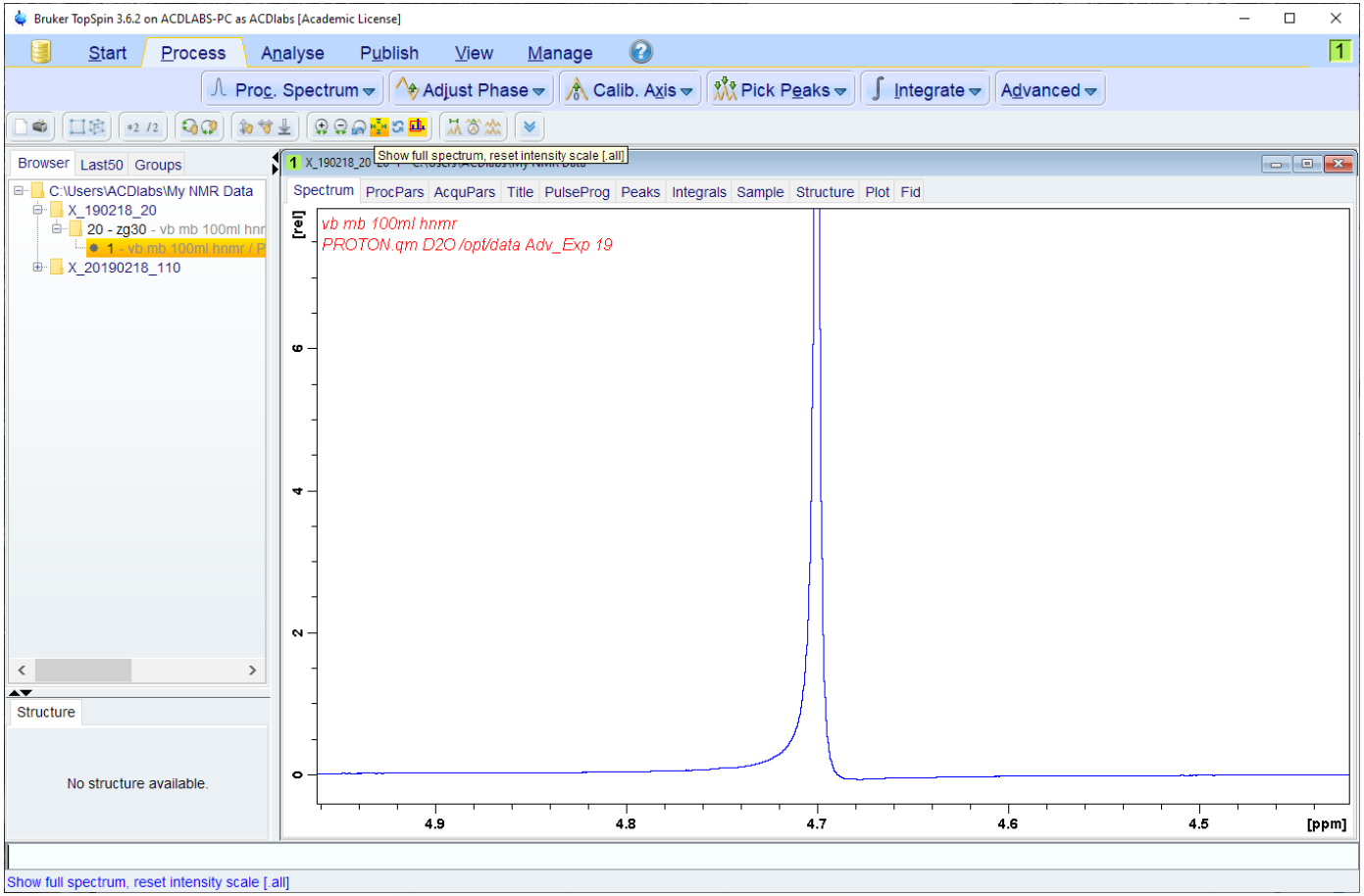
If you choose the Process tab, then the “Adjust Phase” menu, you will get a number of options for correcting the phase.



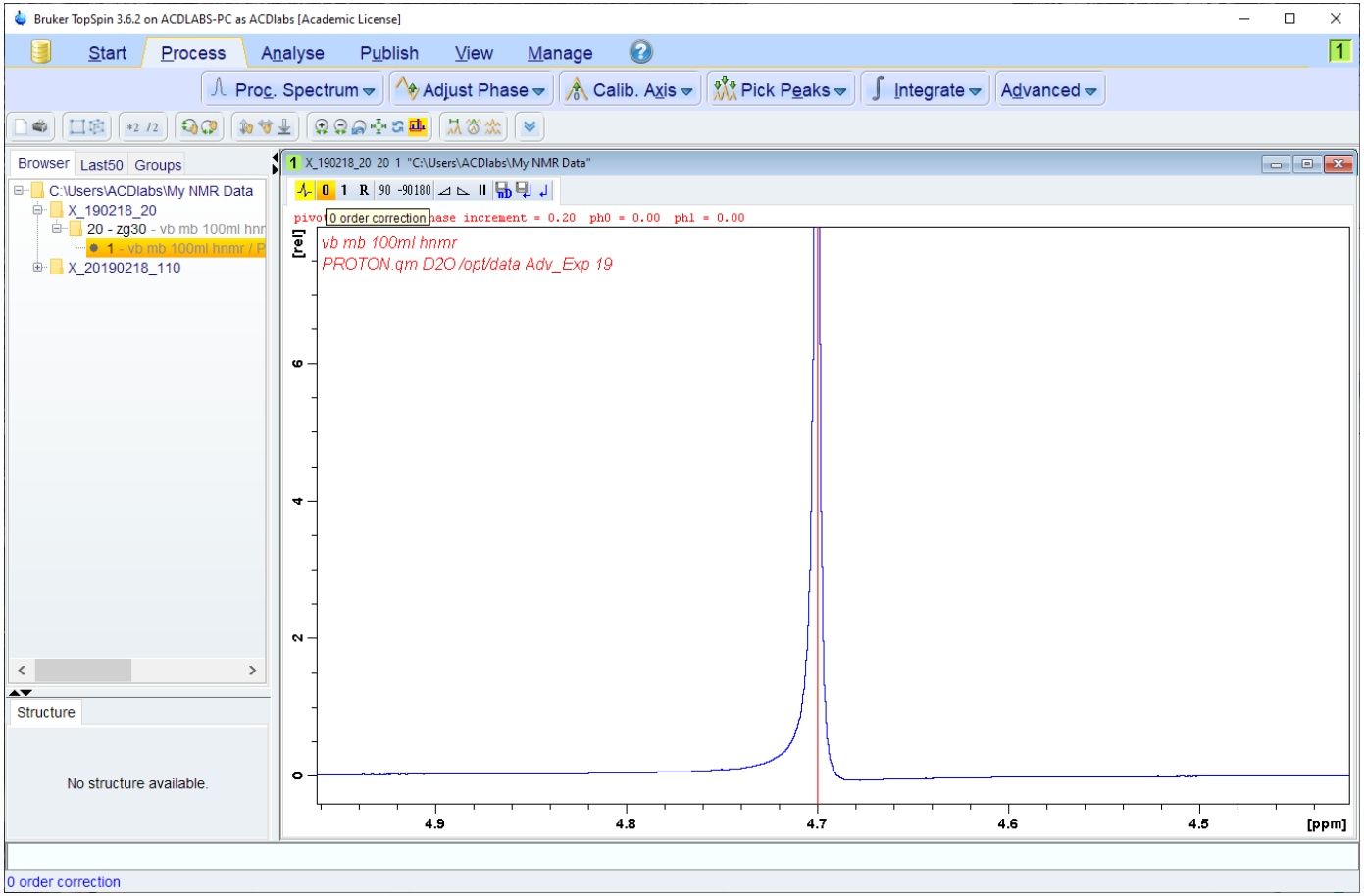
All of the commands can also be typed in to the box at the bottom of the TopSpin window.



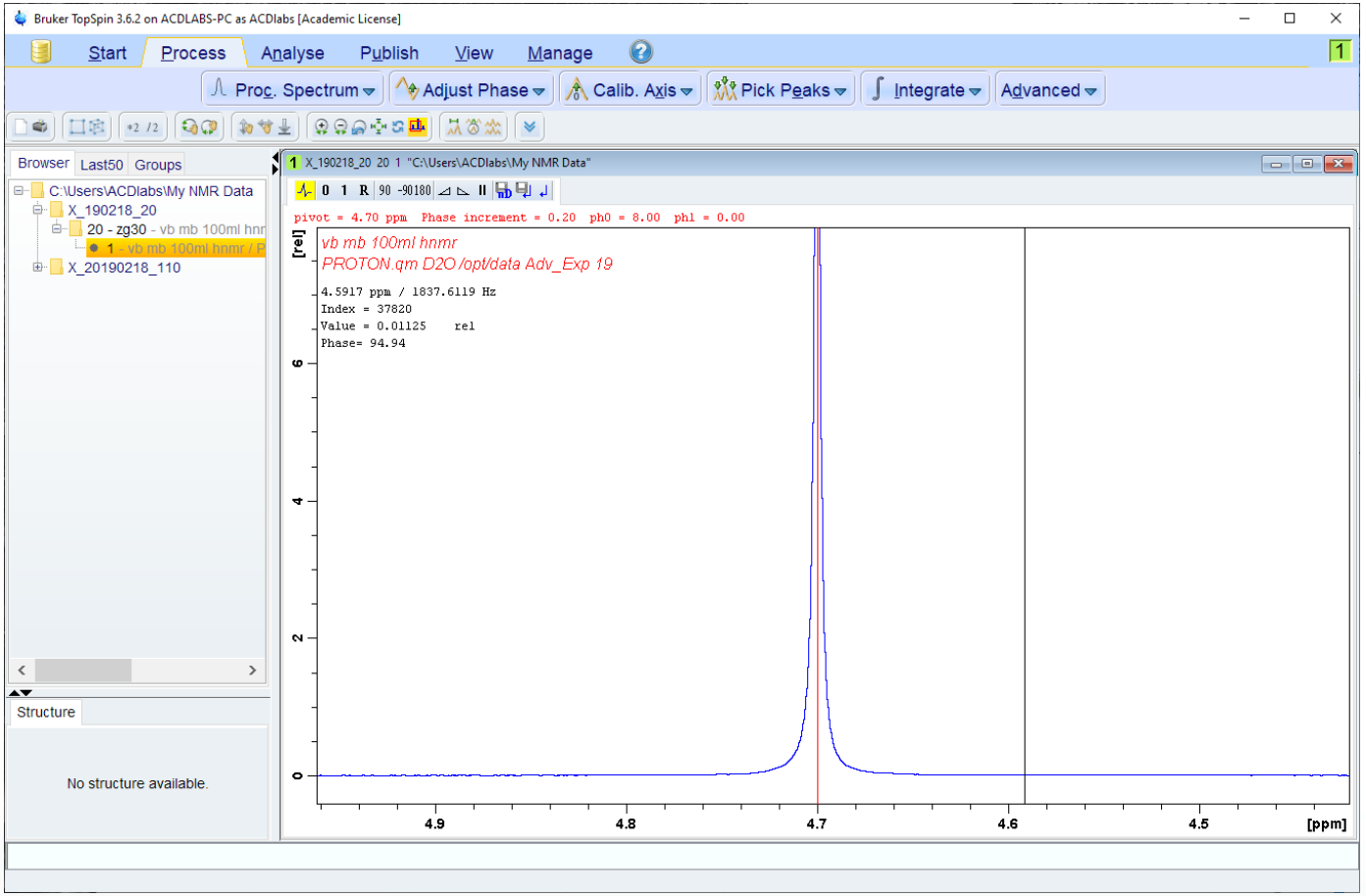
To expand a region of the spectrum click (and hold) the cursor on One side then drag the cursor over the region you want expanded.



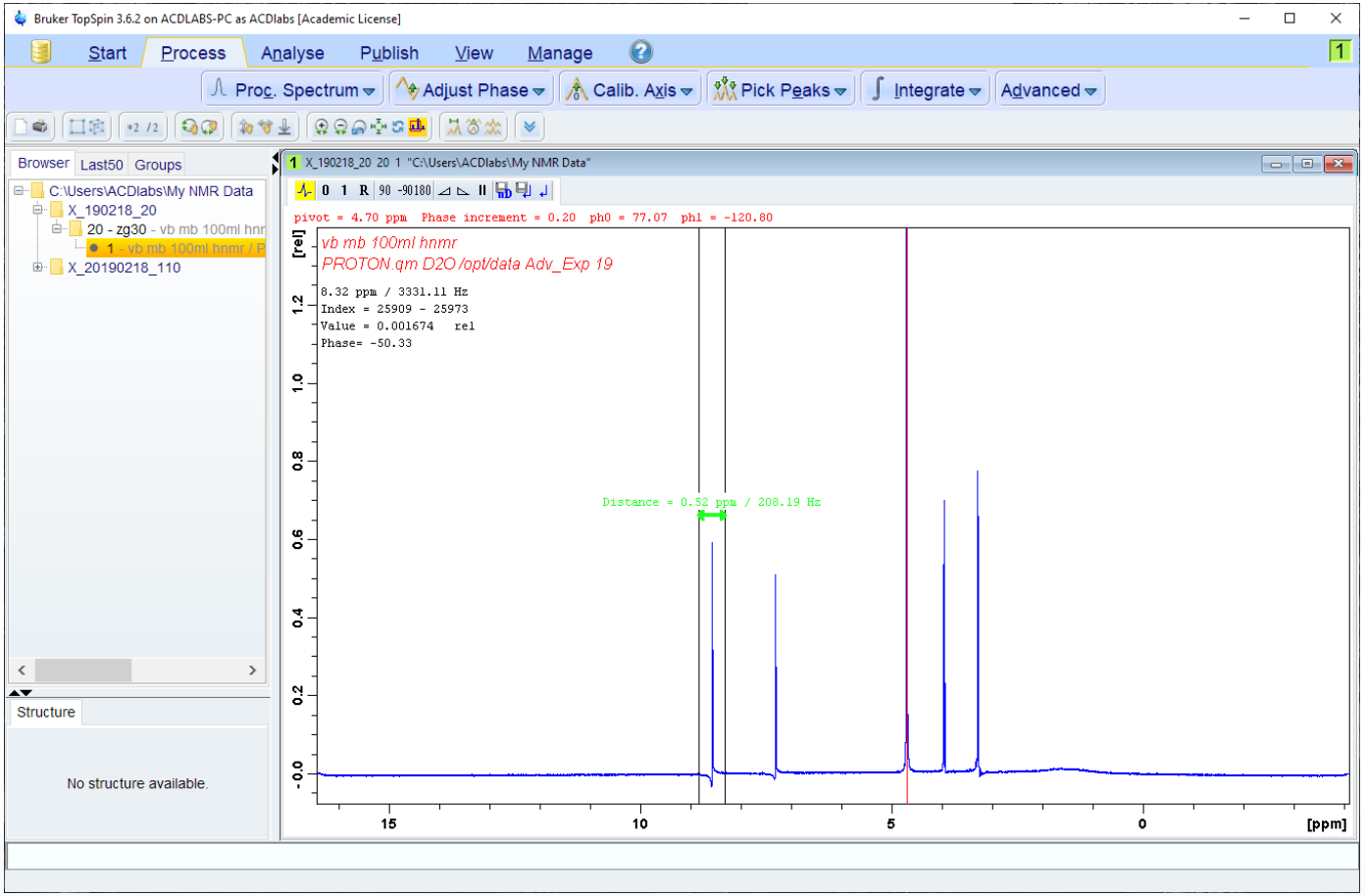
You can adjust the vertical scale with the mouse wheel (or scroll-pad)
When you do, you may find that the phase still isn't quite right.



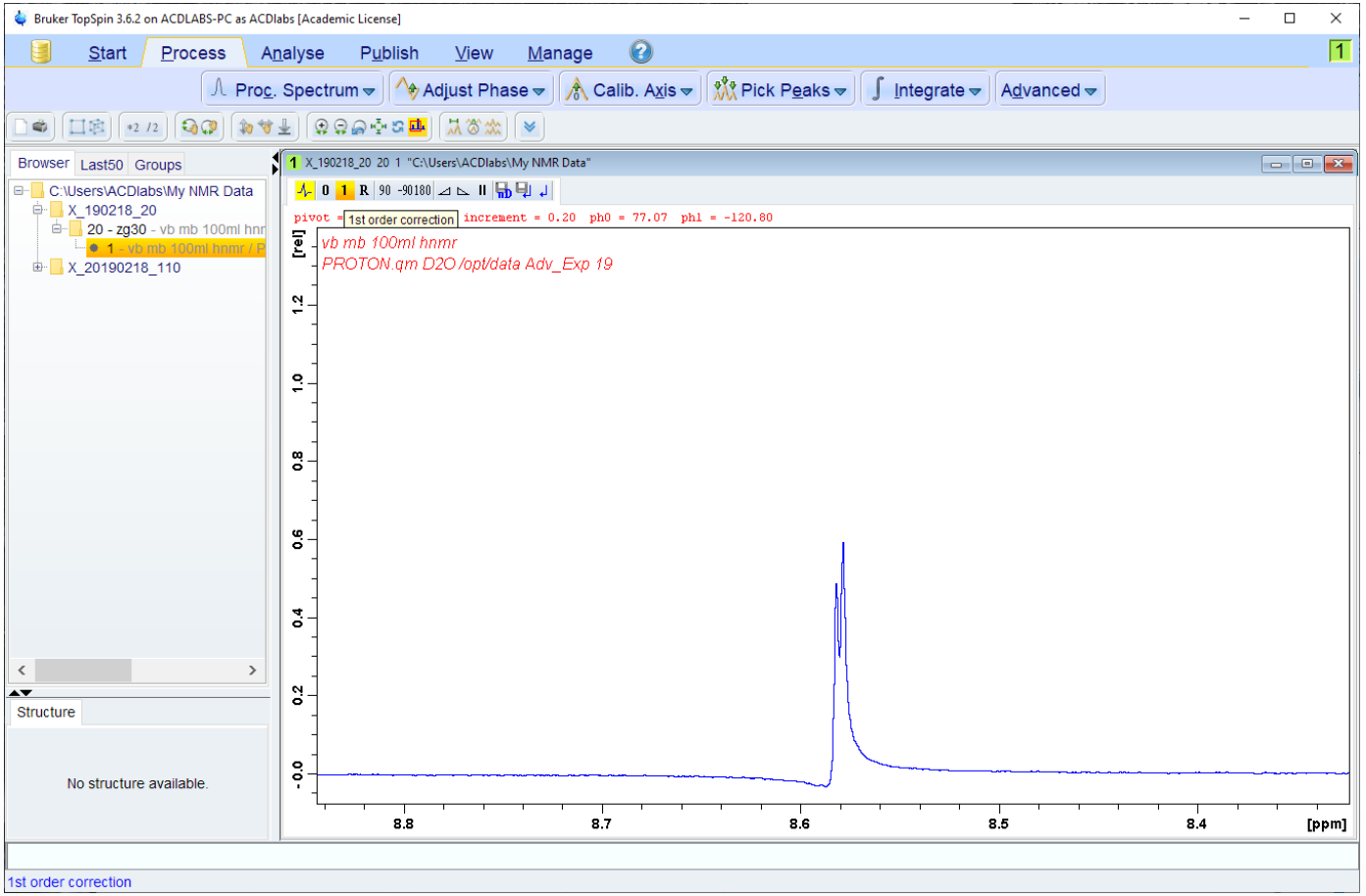
Click on the “Adjust Phase” button to enter manual phasing, then click And hold on the “0” button. Sliding the mouse will adjust the phase.



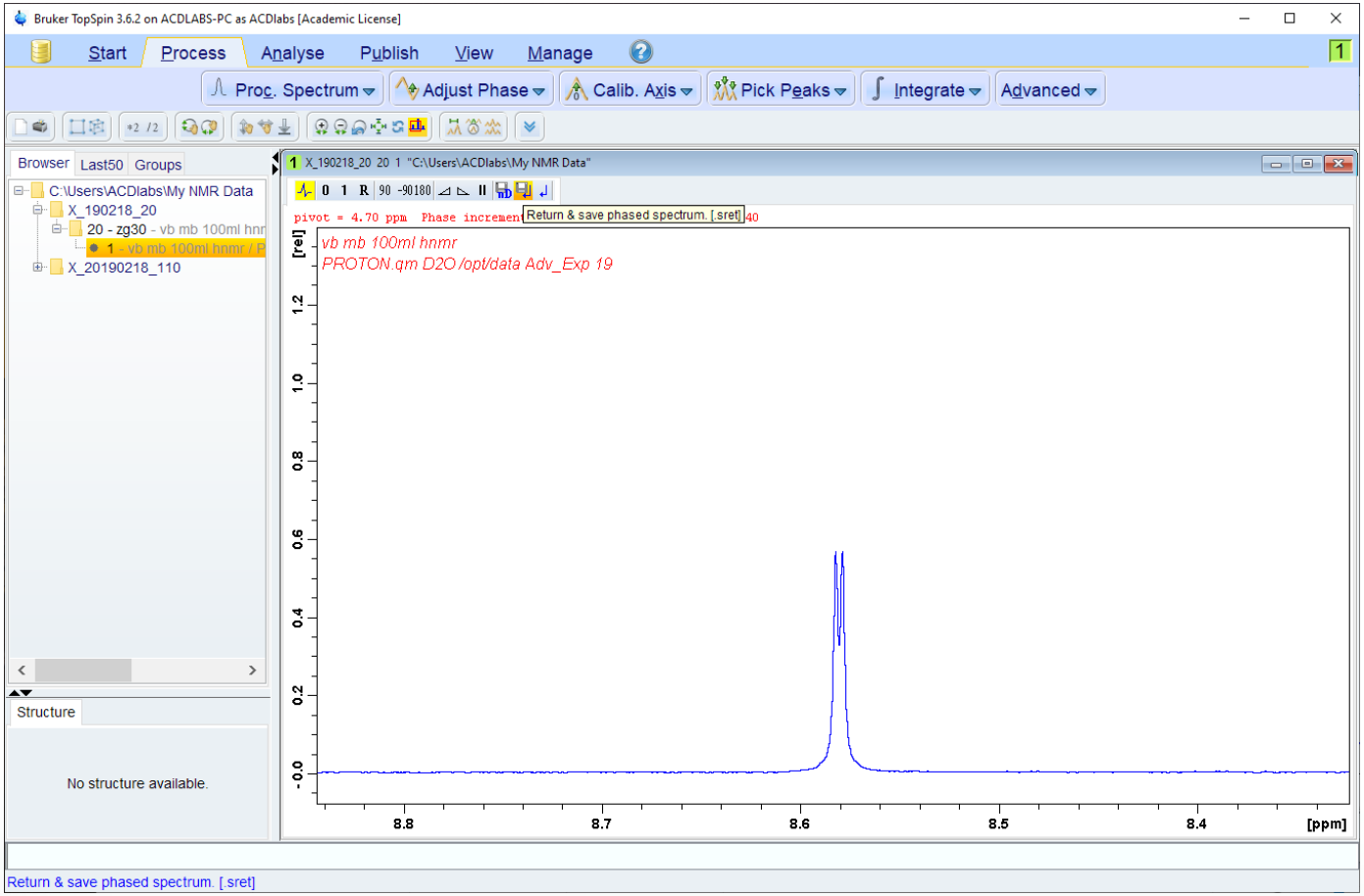
The phase is correct when the baseline is flat on either side of the peak that has a red line on it (referred to as the “pivot point”).



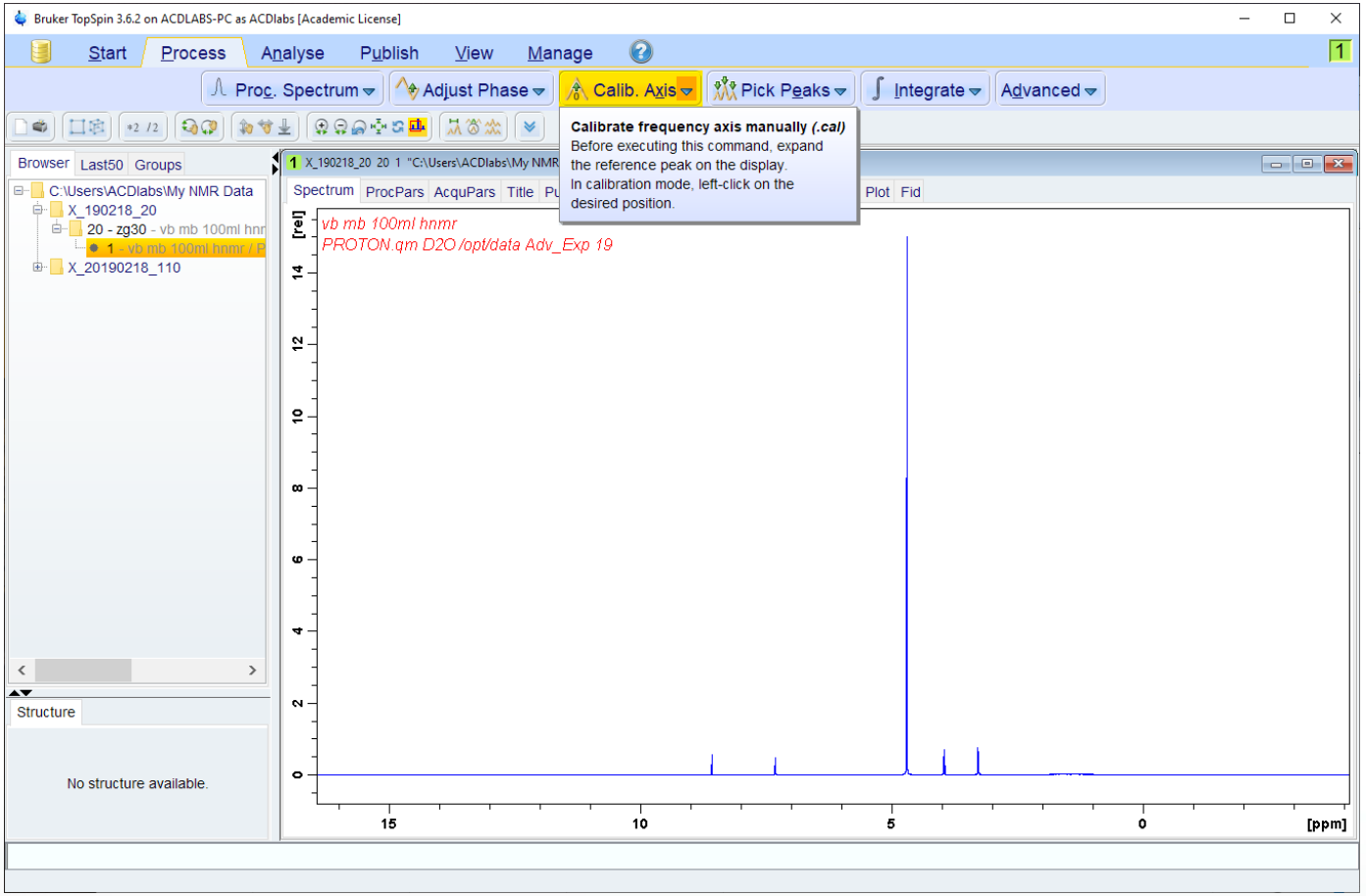
But you may find that lines away from the pivot point are now out of phase. Expand the line furthest from the pivot point.



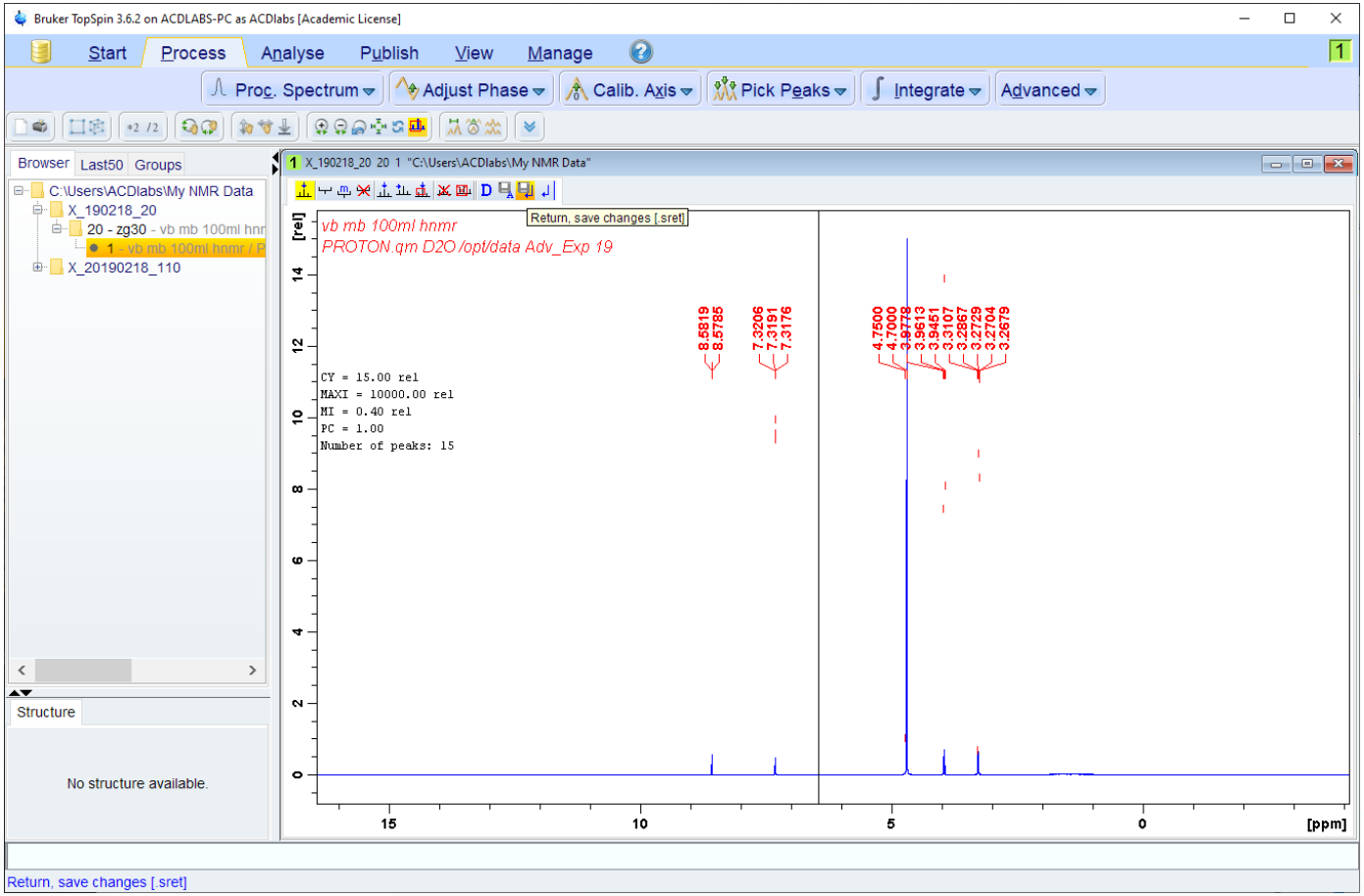
The rest of the spectrum needs a frequency dependent phase correction which is done by clicking/holding/dragging the “1”.



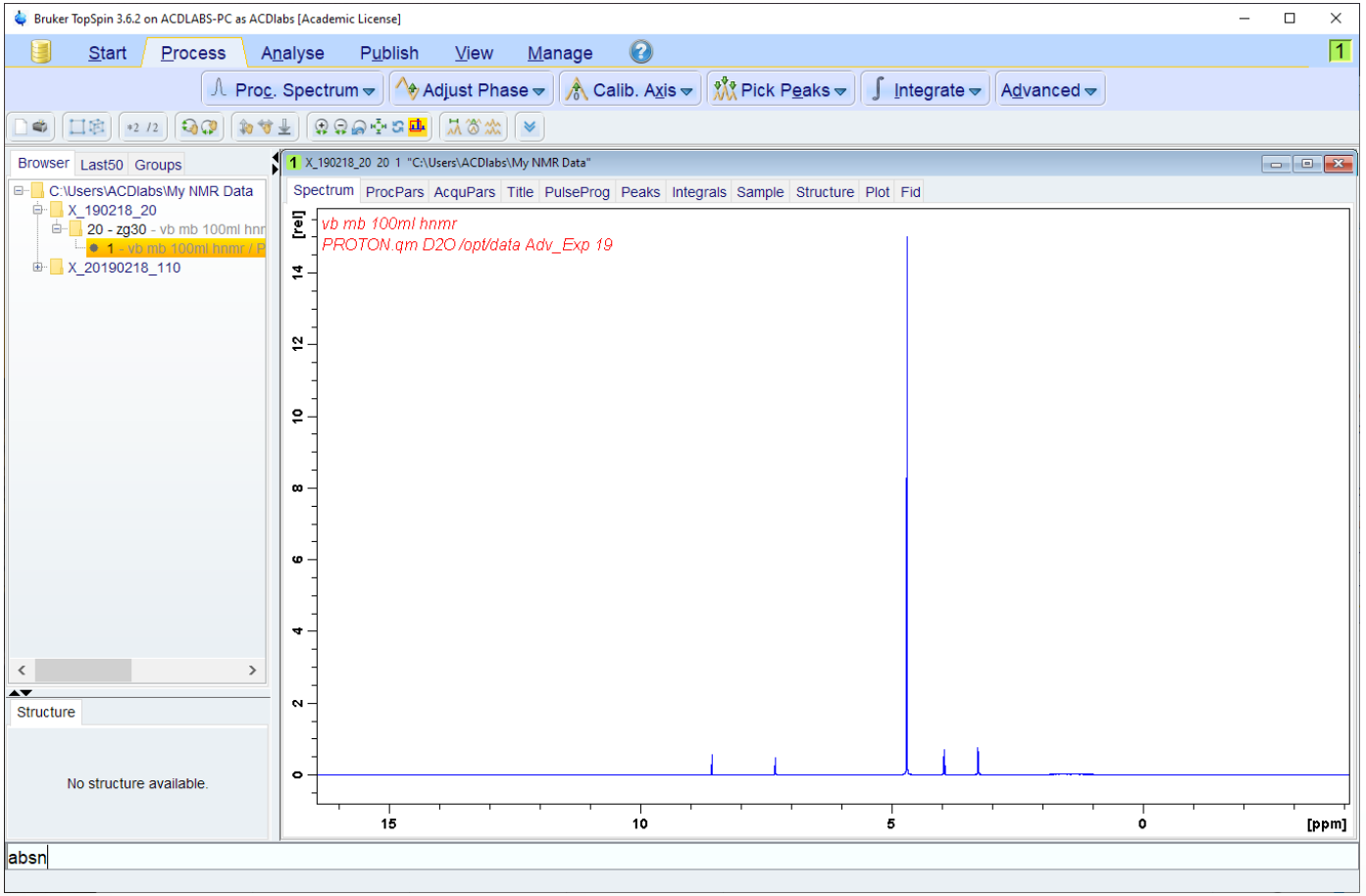
When you are happy with the phasing you need to save the result by clicking on the save icon (looks like a floppy disk).



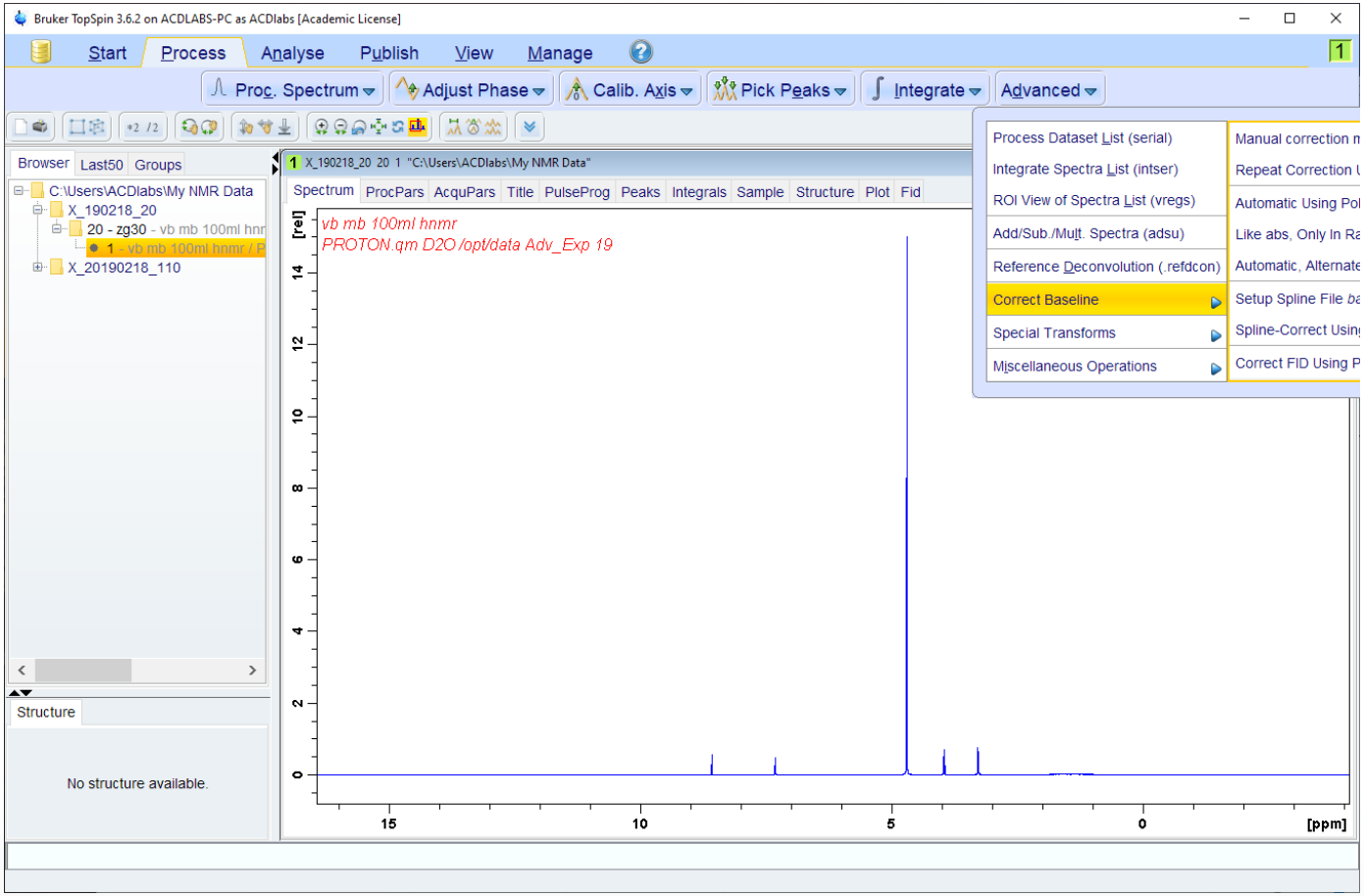
If there is a reference compound (such as TMS) you should now set it to 0 ppm. This needs to be done before anything else.



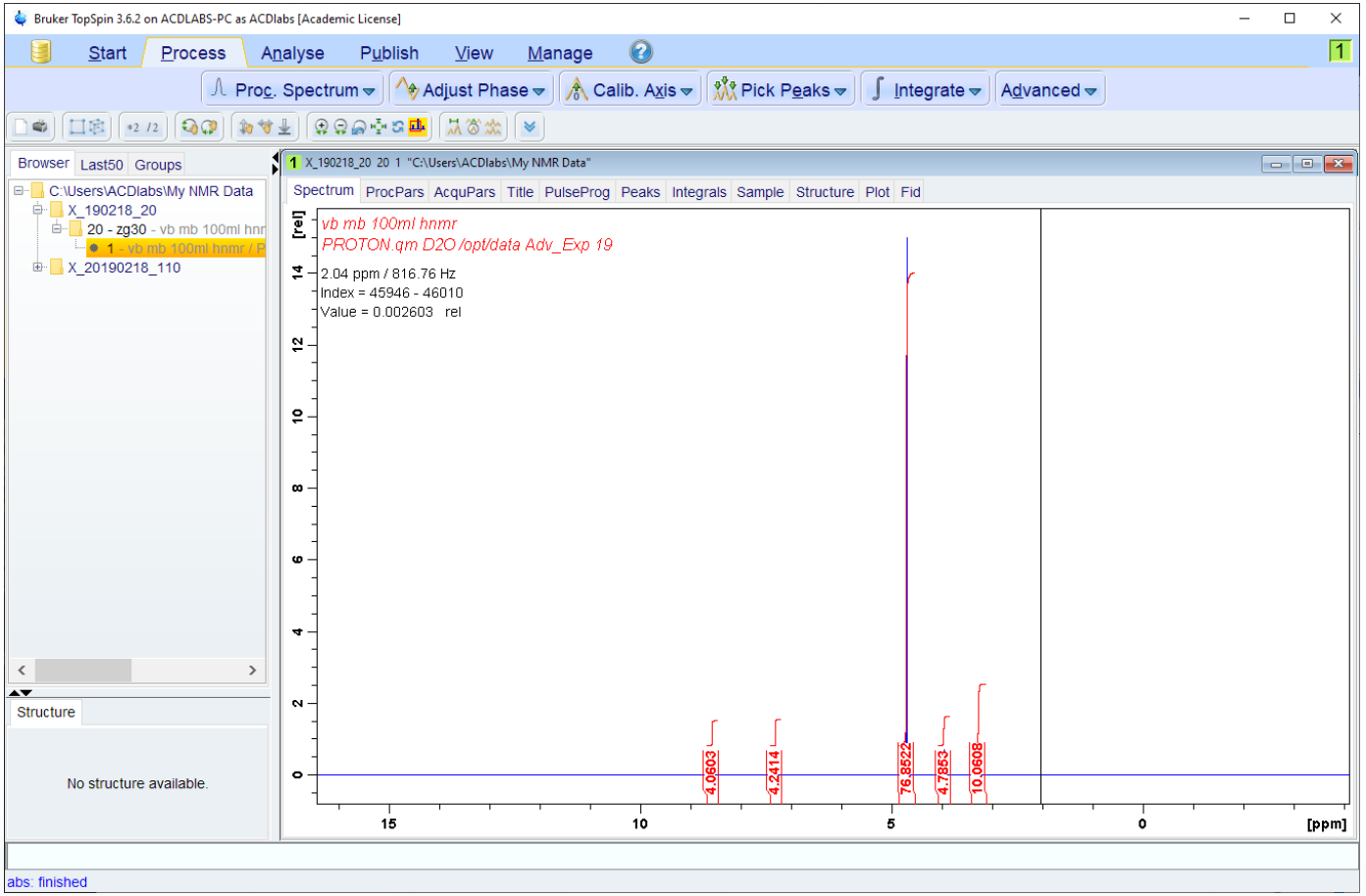
If you select “Pick Peaks” the program will automatically select the Peaks and enter a mode where you can edit the selection.



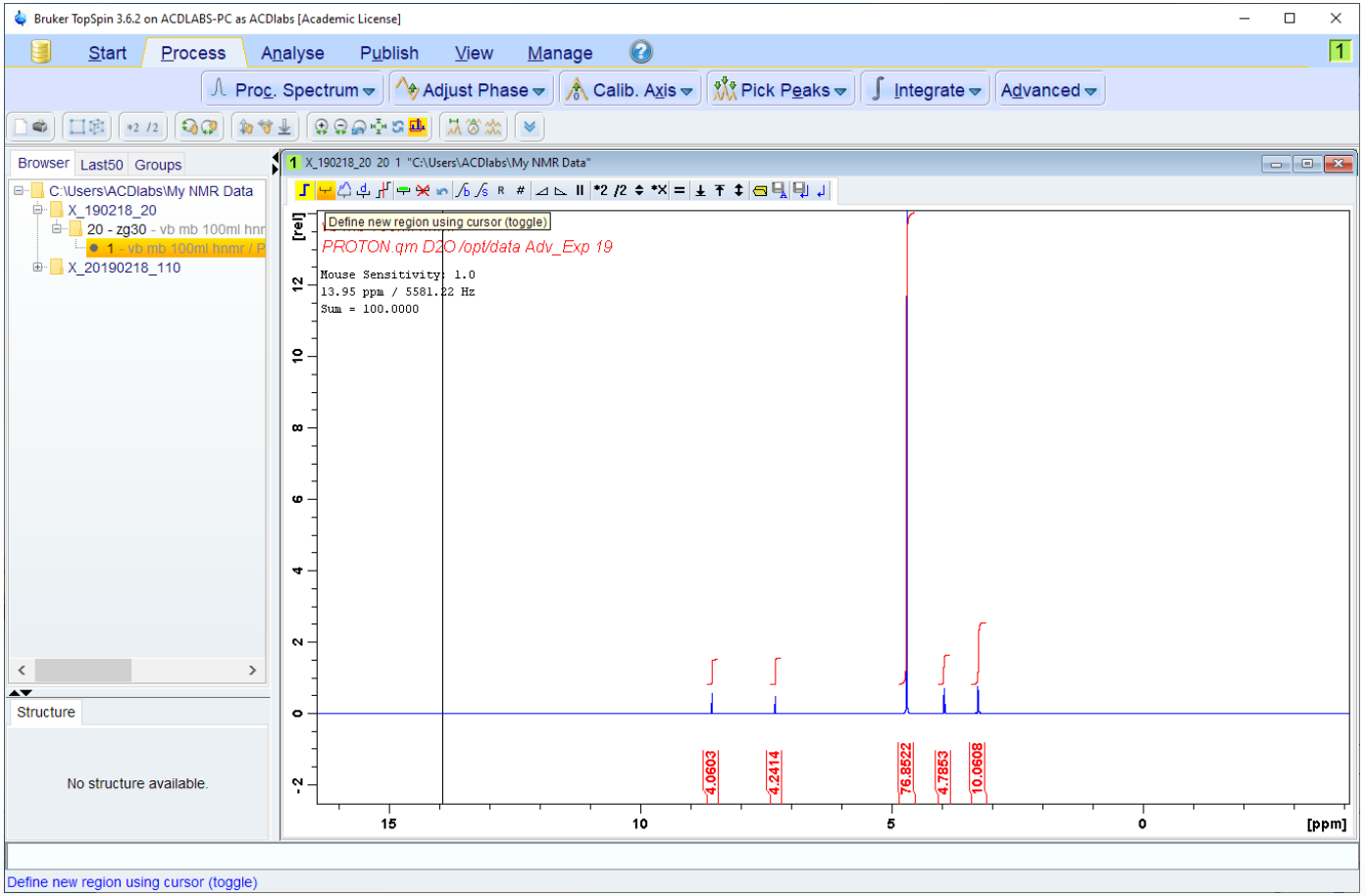
The last piece of processing is baseline adjustment. The automatic version works quite well using the command abs(n).



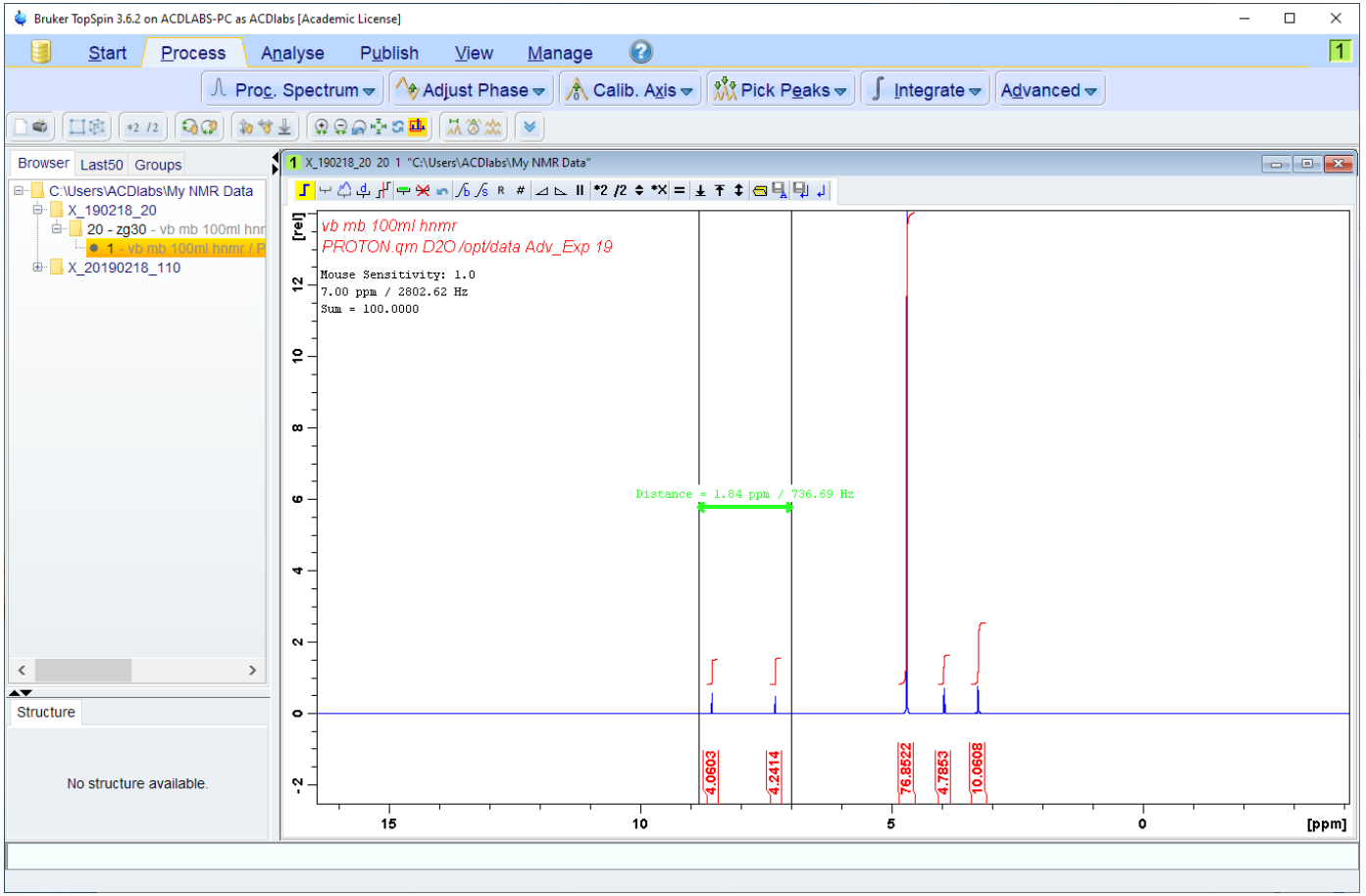
You will find more baseline correction options under the “Advanced” menu. It’s the one place where the work-flow is out-of-order.



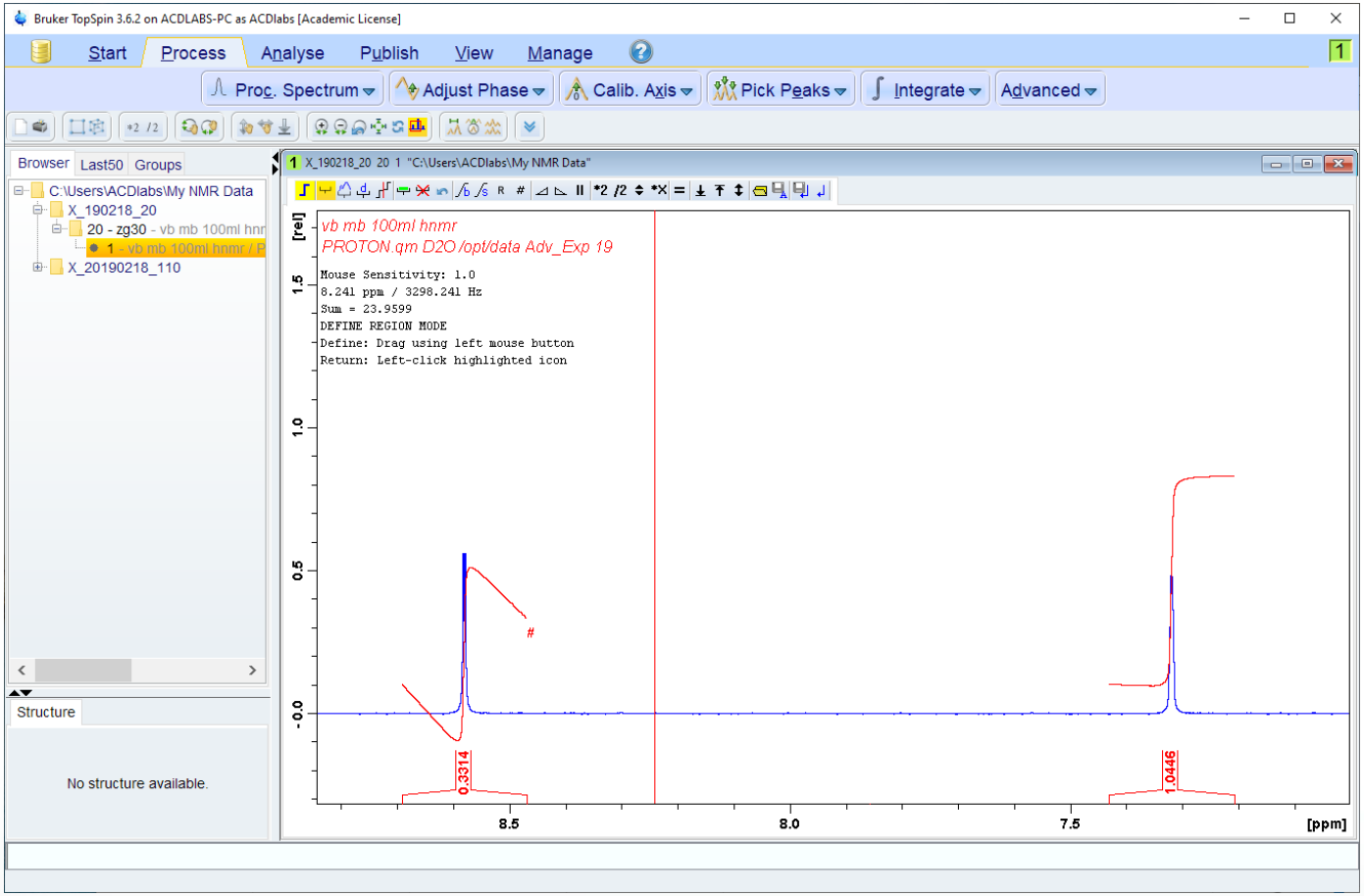
abs will create default integrals, absn performs baseline correction but does not create integrals… leaving you to do so manually.



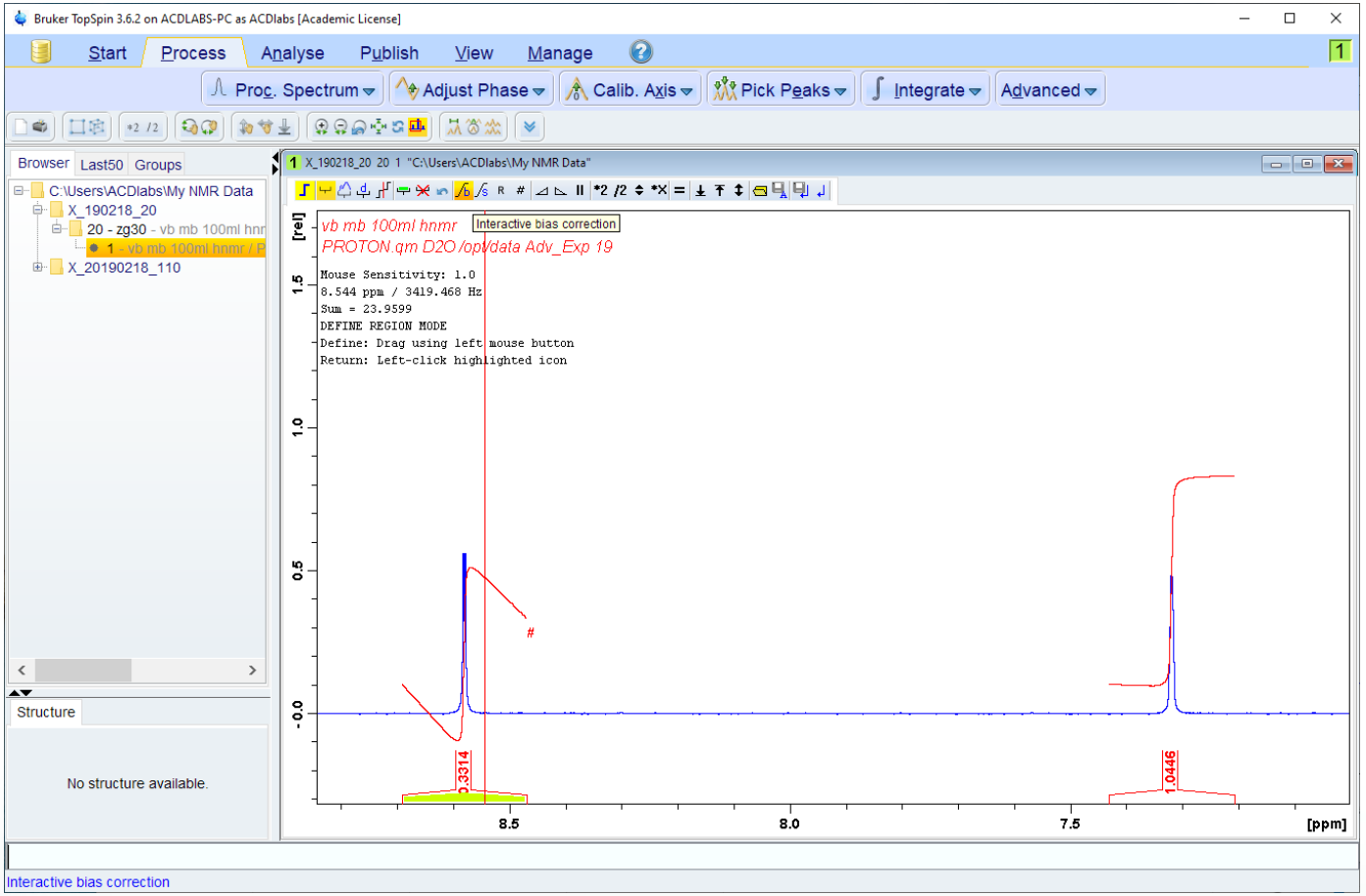
In integration mode. The first icon along enables you to switch between the cursor's integration and expansion modes.



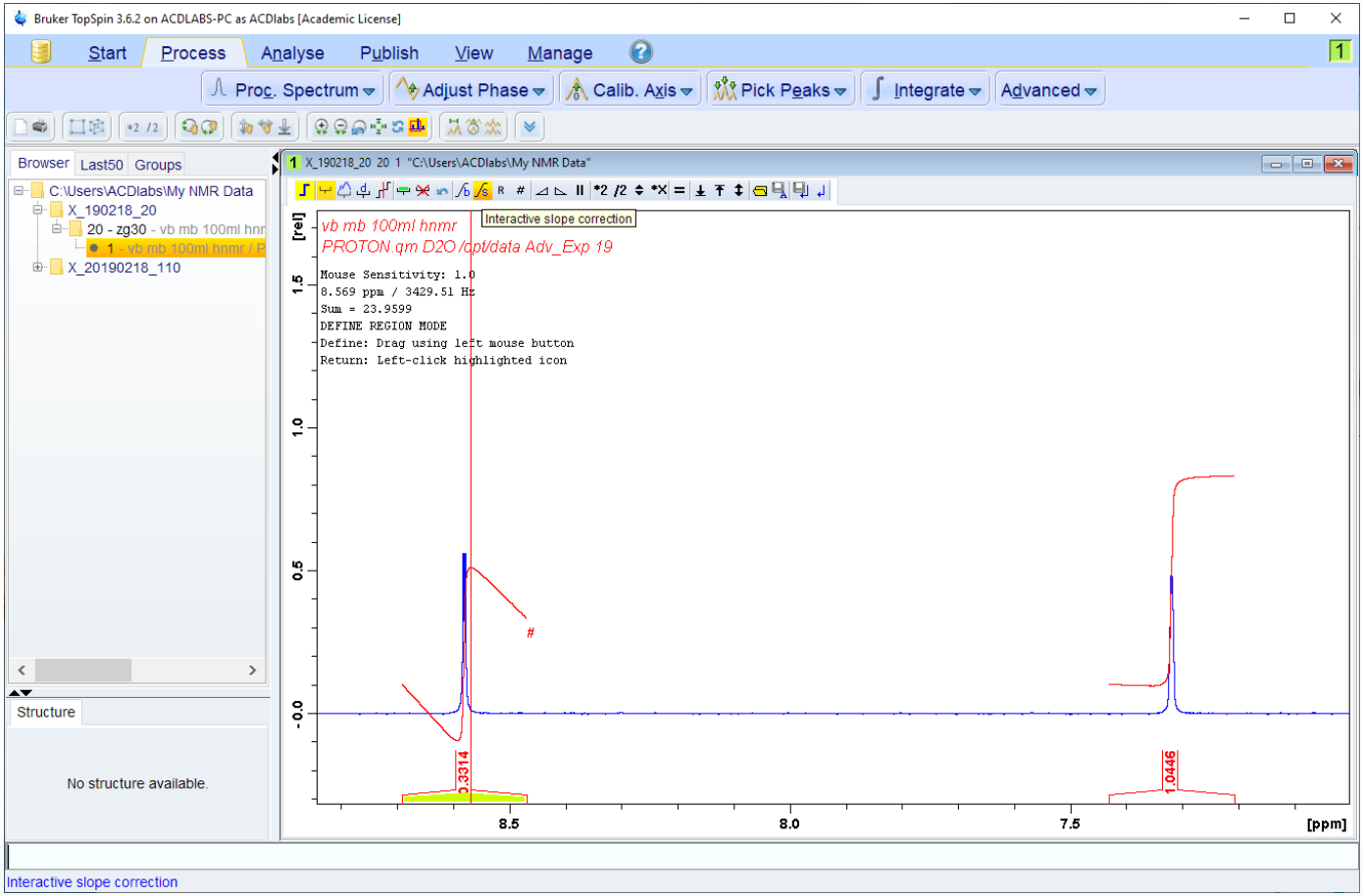
When the icon is not selected you can expand regions of the spectrum as usual.



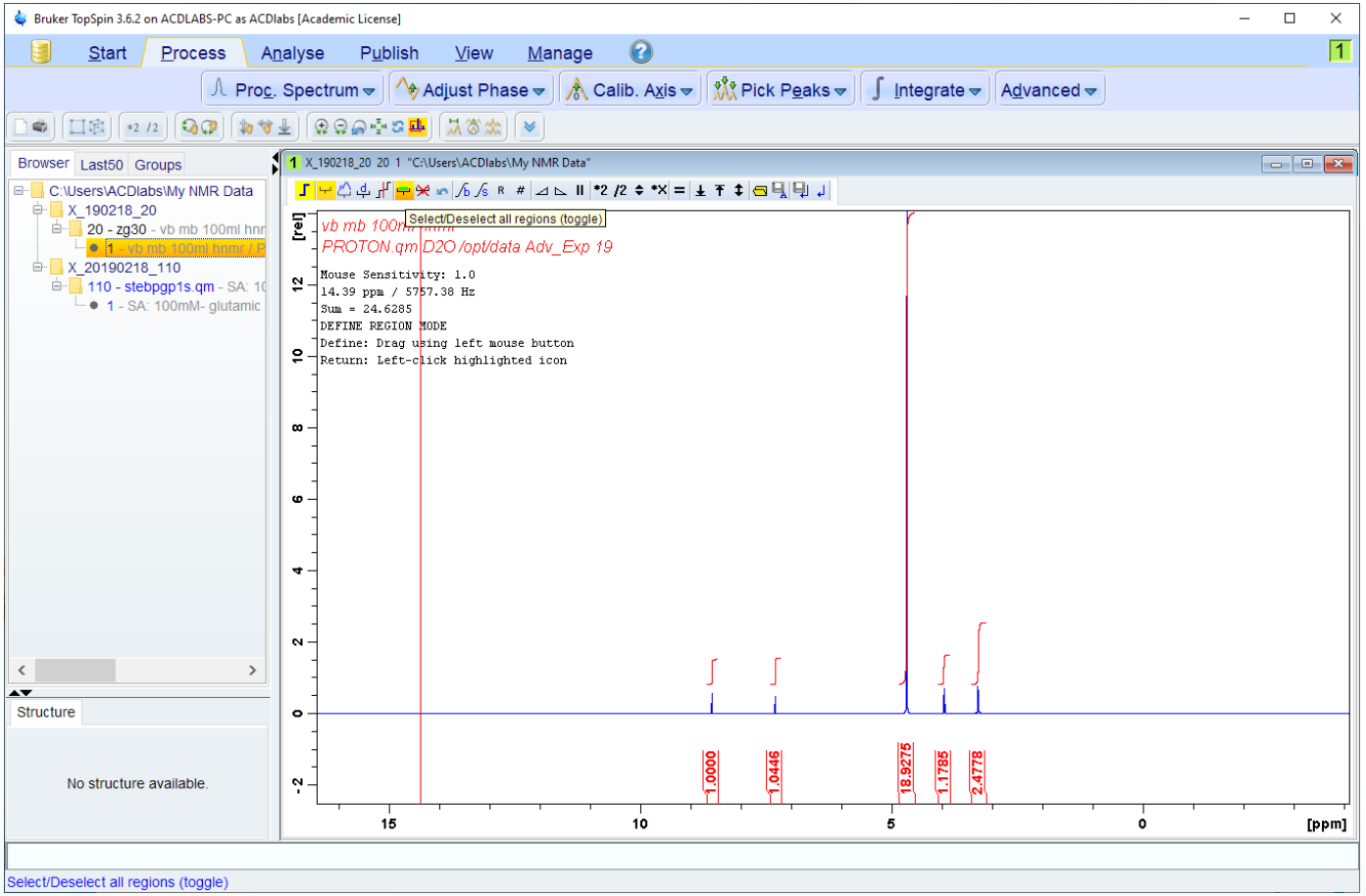
Sometimes a peak (or multiplet) will give a strange looking integral. The slope and bias of that integral need to be manually adjusted.



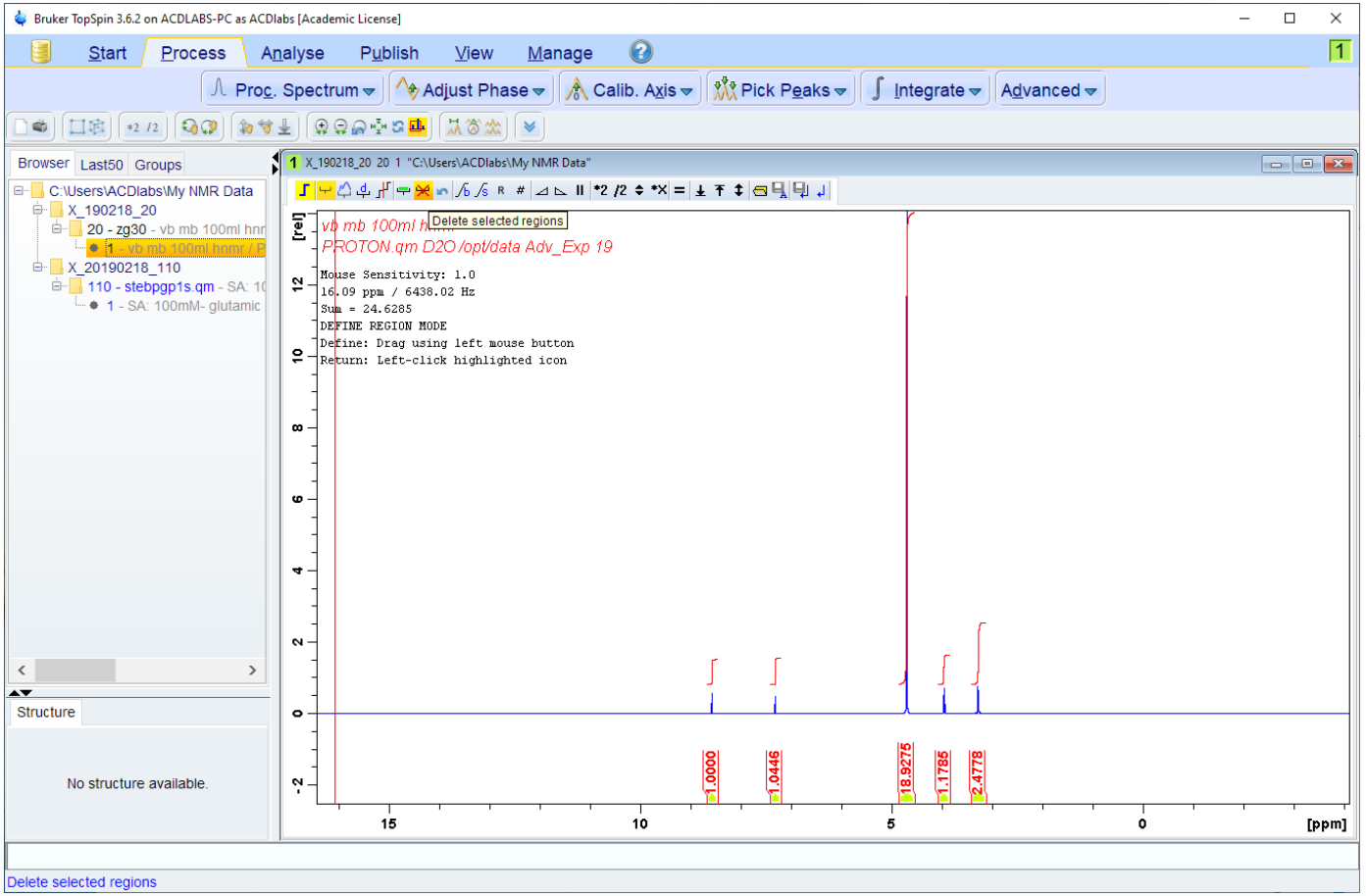
You can select an integral by right-clicking on it (a menu pops up with “Select” as an option. Bias is adjusted with the “b” icon.



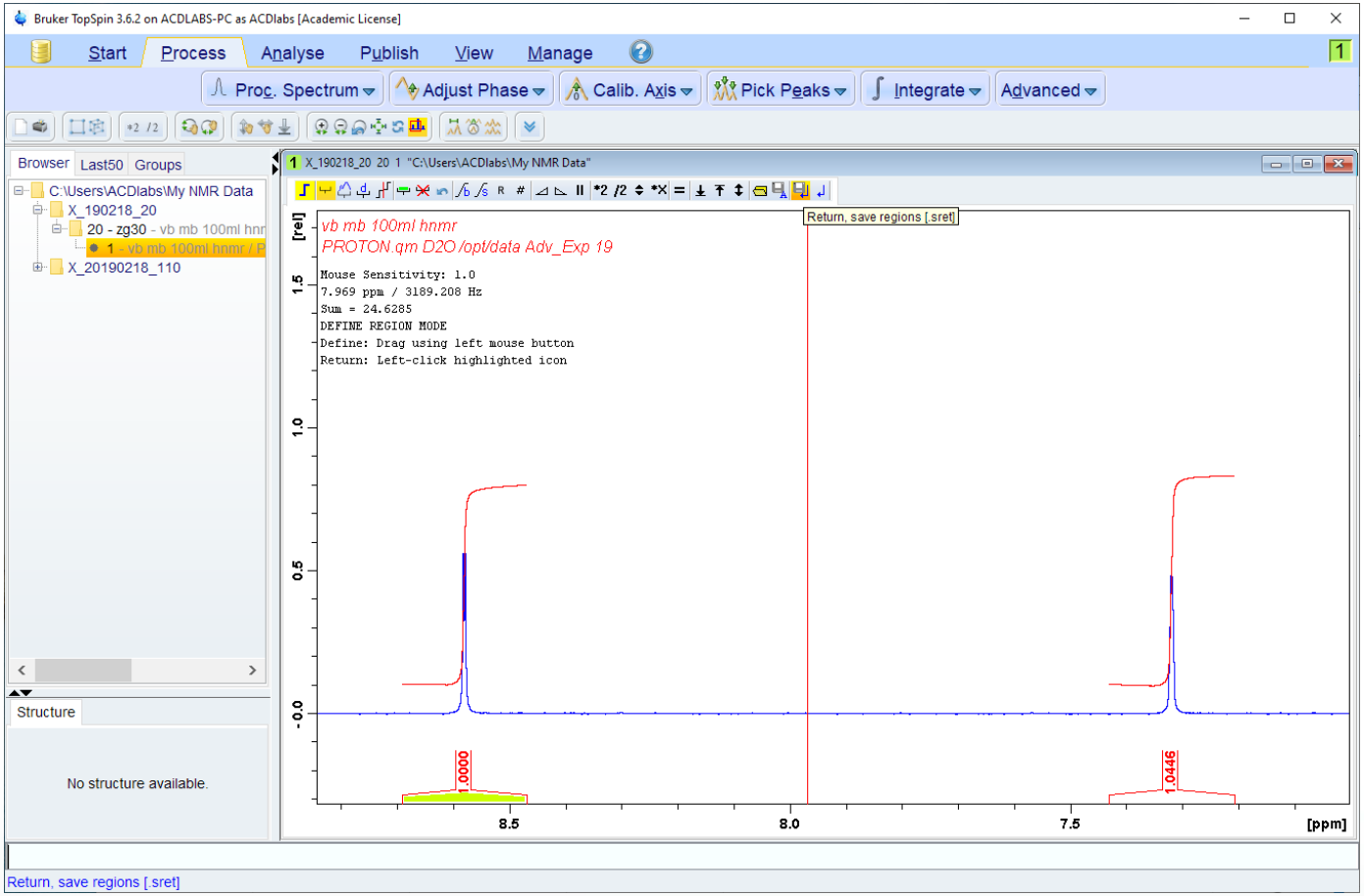
Slope is adjusted with the “s” icon. As with phase correction you need to click and hold on the icon, then drag to make the adjustment.



When you right click on an integral and select it, you can then right--click again to calibrate. There is also a button to select all integrals.



If you select all the integrals, there is also a button to delete them all
Which is useful if you make a mess and want to start again!



And again, as with phase correction, you need to save the results when you've finished.