Taking a proton spectrum in vnmrj.

Login. Click on vnmrj.

On the panel at the left, click Viewport. Move between experiments by typing the experiment no in the Current Workspace input box. If the experiment doesn't exist, it will be created.

In the Experiments drop-down menu at the top of the window, select Setup new parameters for Proton.

In the Start – Shim panel, click Read default Shims. In the Standard panel, specify the solvent and label the sample in the Comment box.

Click Find zo. When it is done, check that the sample is locked. If not, turn the lock off and then on, or, if needed adjust the lockpower and lockgain. Optimize the lockphase for the maximum lock level.

Click Gradient Autoshim.

When this is done, move to the Acquire folder and adjust the spectral window, acquisition time, relaxation delay and number of transients, then click the green Acquire button.

When the acquisition finishes, the FID will be processed automatically. This includes autophasing, finding the integral regions and baseline correction.

Go to the Process folder in the Default panel. The chemical shifts are already referenced to the solvent. You can set the reference to another peak by typing in the input box what chemical shift you want at the cursor.

On the menu at the right of the display area select the integral dispay 'partial'. At this point, integral regions are defined automatically. Click BC correct at the bottom, then Clear Integrals. Now use the Integral resets button on the right to define the regions that you want. Click the spectrum icon on top to get out of defining zeroes for the integral.

Move to Integration, select single peak and input the value you want for the integral under cursor.

Click on the Save icon on top of the window, move to your home directory, and create a directory for the project, then for the compound. Select the directory path at the bottom of the dialog window and copy it with CTRL-C. Then type *h*, to save the proton spectrum.

Move to the Chemical Shifts panel, and CTRL-V in the change directory to: input box. Your current directory now is the one where you saved the spectrum.

Move to the CS Plot panel and click Standard Proton. In the file name input box type a name for the printout, say h, then click make.pdf. After that, you can make a .png file, to be taken into PowerPoint.

From the File menu on top of the window, select Exit vnmrj. Click on System at the top of the screen, and drag down to logout, and then confirm that you want to logout.