NMR Operation without Sample Changer

1. Wipe the exterior of the NMR sample tube using a clean Kimwipe to remove fingerprints and other deposits on the tube.

2. Carefully slide the sample into the *spectrometer* and proceed to sample analysis.
   The sample temperature will stabilize within 1-2 minutes, ensuring optimal performance while you are selecting/verifying the parameters for your NMR experiment:

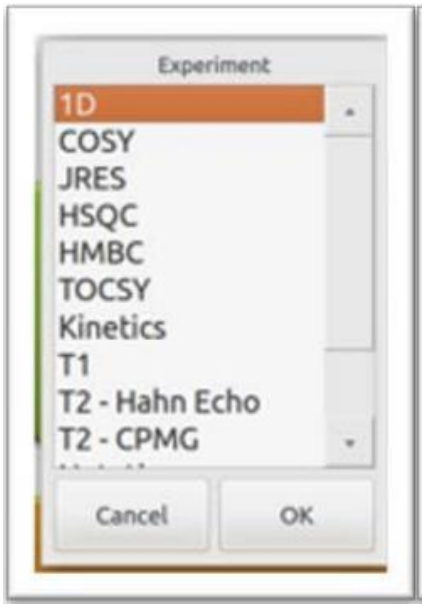
Setting up basic parameters

- **Observe nucleus** – This button lets you choose the nucleus you wish to observe [1H, 13C, 19F, etc.]. Select the desired nucleus on the popup menu, followed by OK to confirm the selection.

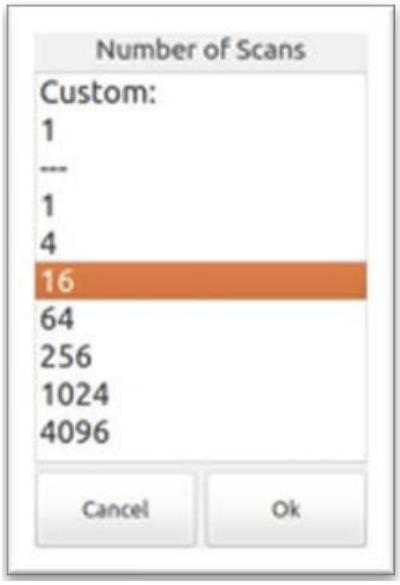
- **Lock nuclei** – The lock nucleus is kept at the standard deuterium 2H for samples prepared in deuterated solvents. The OK confirms the selection.

- **Solvent** – Click the solvent button for a popup menu listing NMR solvents. Select the appropriate solvent, followed by OK to confirm the selection.

- **Experiment** – Upon hitting this button, a popup window will appear with various 1-D and 2-D experiment options available. Select the appropriate experiment and the OK button to confirm.



- **Number of scans** – Upon hitting this button, a popup window with a list of the number of scans [in multiples of 4] can be specified depending on the desired spectral output.
  For a 1-H proton NMR 4 or 16 scans should give you a decent output.



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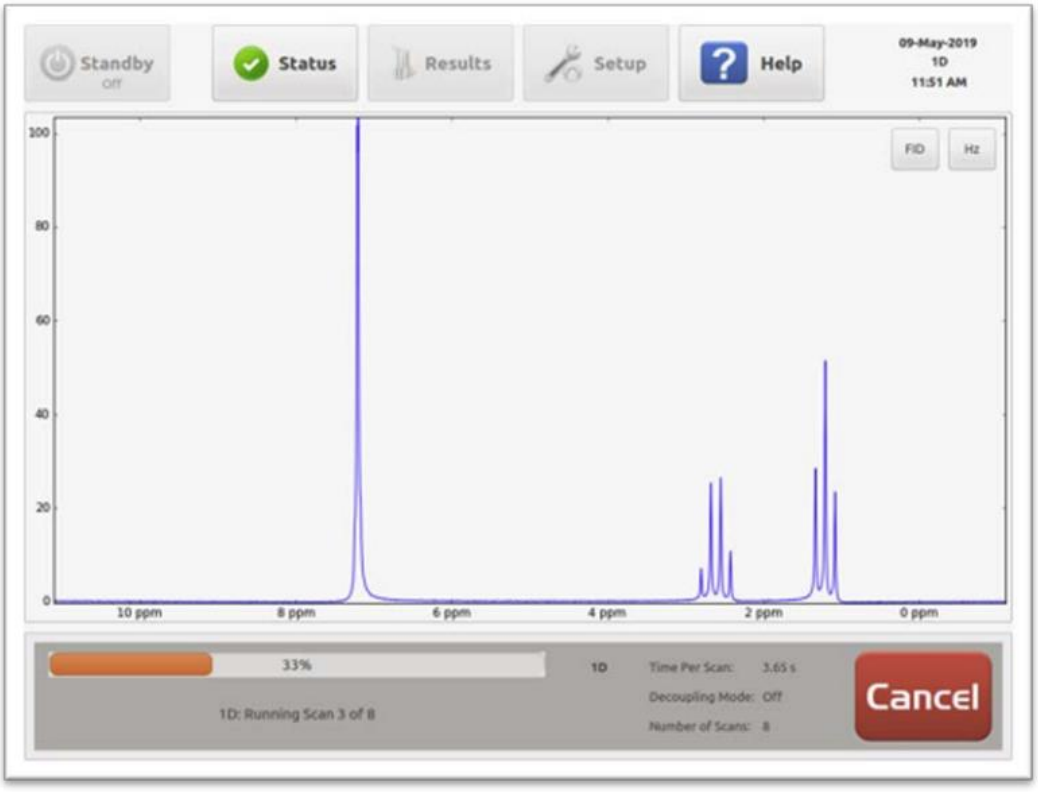
NOTE: The instructor or technician will preset experiment settings/acquisition parameters depending on the experiment and the sample(s) being analyzed.

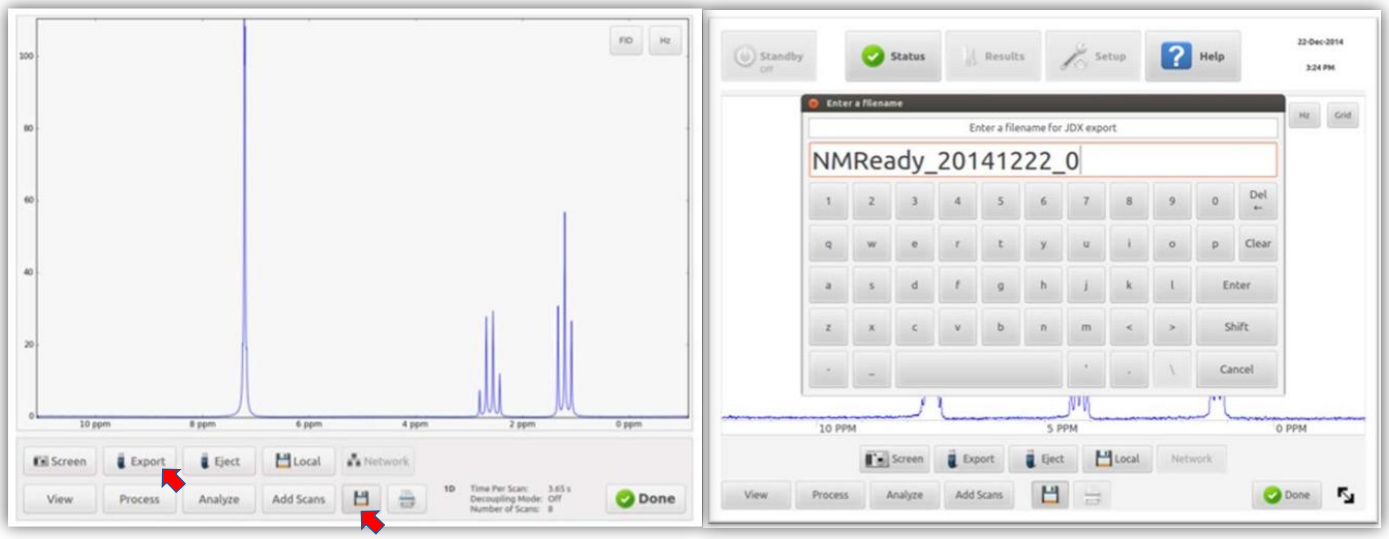
Once the basic parameters are set, hit the **GO** button to initiate the experiment.

After the first scan, the *Fourier-transformed* spectrum will be displayed and updated with signal-to-noise improvements with every additional 4 scans.



Saving the file

Upon hitting the disk icon on the screen, several saving options will appear. Click the export option to save the file to a USB key (thumb drive). Use a unique filename for each group. The default file format will be the *file*.dx format. Click the eject button to remove the thumb drive safely.



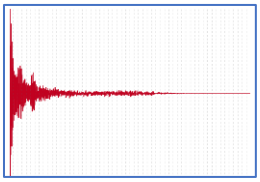
Remove your sample tube after the data has been saved.

On your lab computer, open the web browser, navigate to – www.nmrium.org/nmrium, and drag your xxxxxxxx.dx file into the browser to begin spectral processing.

NMR Spectrum Processing with NMRium

1. Open your web browser and navigate to www.nmrium.org

2. Drag your NMR file (xxxxxxx.dx) into the browser to see the raw *FID:*
(Skip to Step 7, if you already see a *spectrum*.)



3. Click the **Apodization** button to reduce the noise.
Set **Line Broadening** to 0.5 and click the Apply button.

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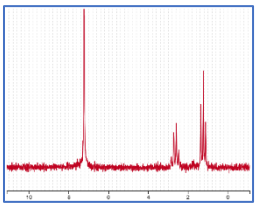
4. Click the Zero Filling button to improve the resolution.
Increase the **Size** to 32K and click the Apply button.

5. Click the **Fourier Transform** button to convert the FID to a *Spectrum:*



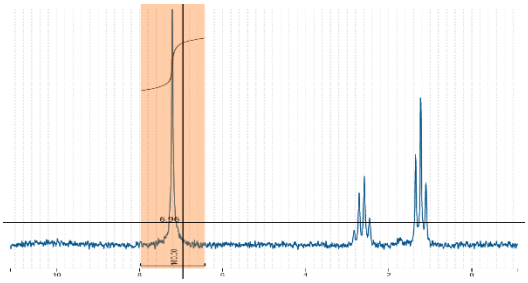
6. Click the **Phase Correction** button.
Change from Manual to **Automatic** and click Apply.

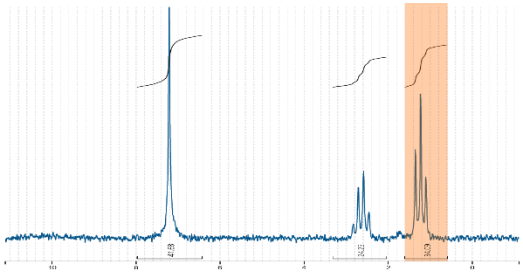
7. Click **Baseline Correction** and click Apply to straighten the baseline.

8. Click the **Peak Picking** button and click Apply to display the peak positions.

9. Click on the number above the TMS calibration signal and change it to "0".

10. Click the **Integration** button.
While holding the SHIFT key on the keyboard, click and drag the mouse pointer across the first signal. This will define the first integral region. Repeat for the other signals in your spectrum.





11. **Export** your finished spectrum as a **PNG image**.