

VnmrJ 3 QUICKSTART GUIDE

Collecting an NMR Spectrum

NMR SOFTWARE

The Measure of Confidence



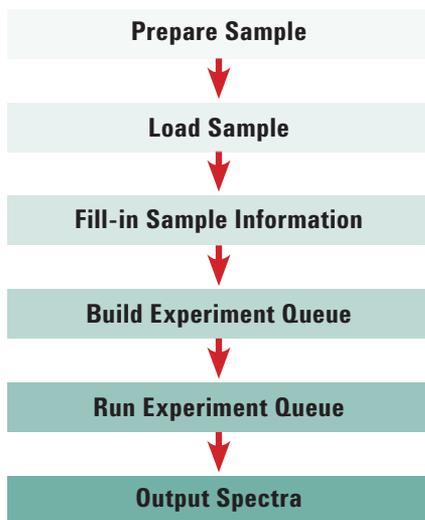
Agilent Technologies



Collecting an NMR spectrum requires just a few simple steps:

- The sample must be dissolved and then transferred into an NMR tube.
- The NMR tube must be inserted into a spinner turbine, positioned at the appropriate depth, and then placed into the magnet.
- The spectrometer must be supplied with information appropriate to the sample, such as notebook numbers and the solvent used to dissolve the analyte.
- A list of experiments to be performed must be selected.
- The spectrometer can then automatically optimize conditions before collecting and saving the requested data.
- The completed data can be processed and displayed as desired. That display can be used to generate output in various formats.

This QuickStart Guide will lead you through these tasks with just a few easy mouse clicks.

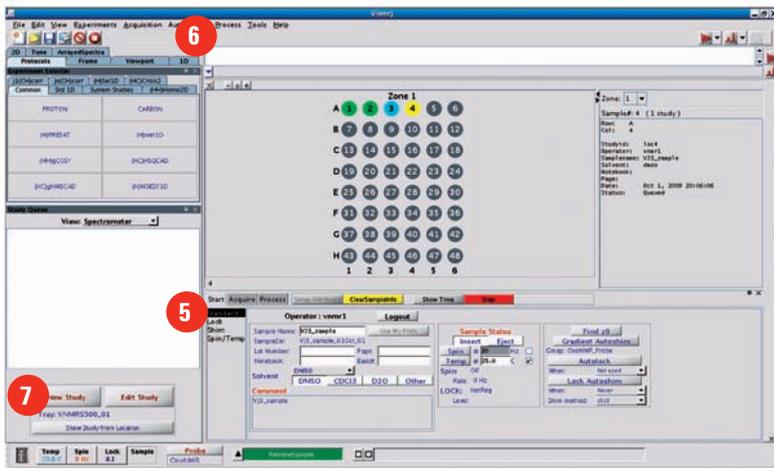
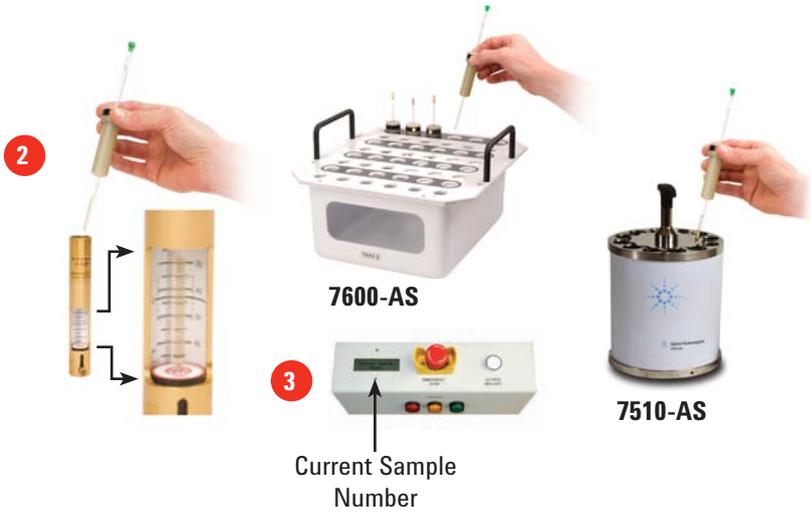


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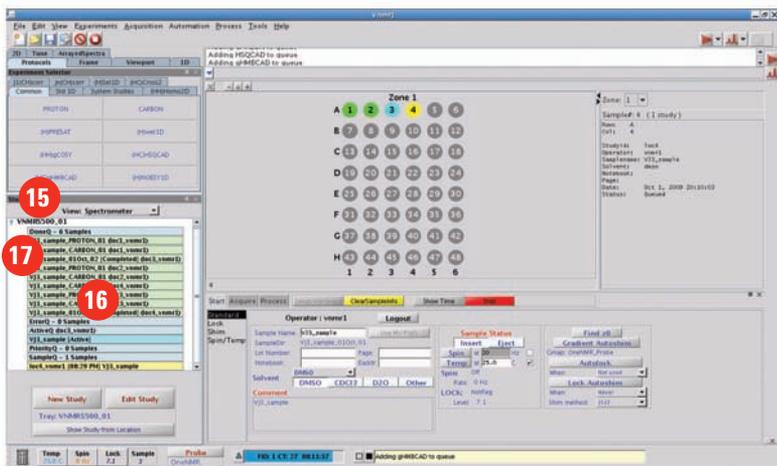
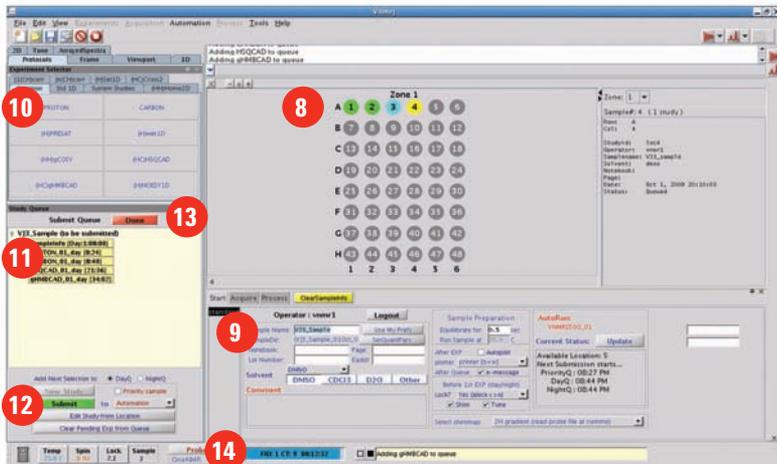
Collecting data on systems without a Robot Sample Changer pages 9 - 15

Collecting data on systems with a Robot Sample Changer

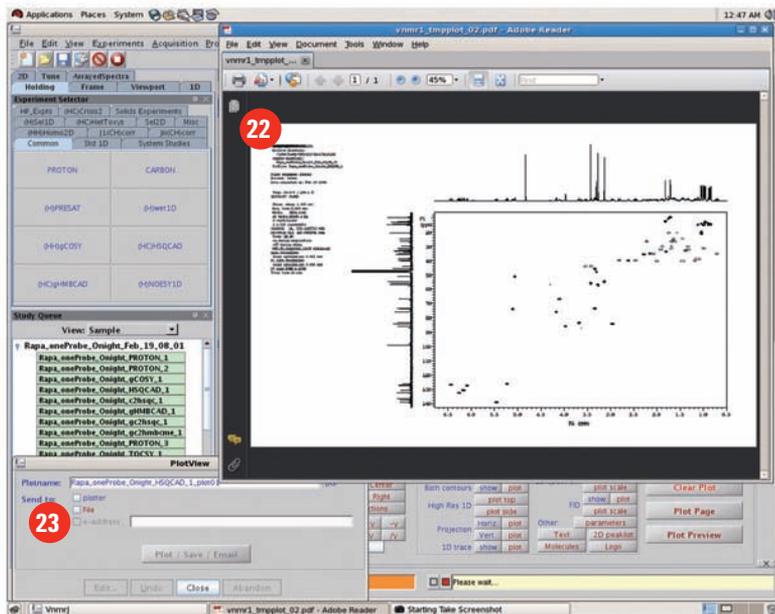
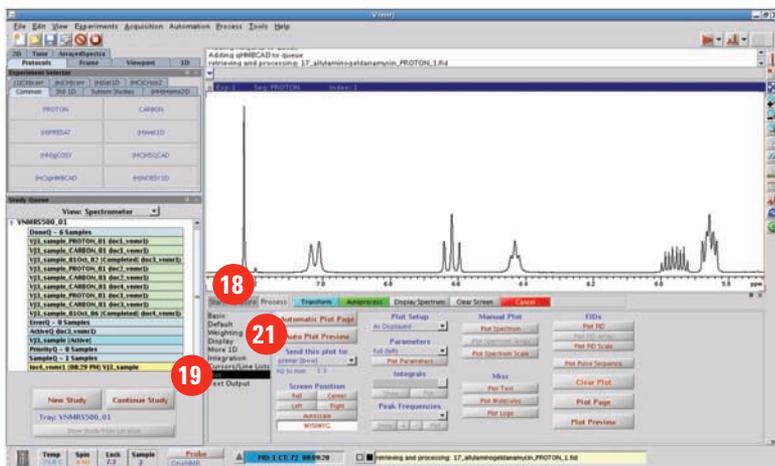
1. Prepare the NMR sample by dissolving the analyte in an appropriate deuterated solvent. Any concentration between ~1 mg/mL and ~50 mg/mL should work well if the sample is completely dissolved. Transfer between 600 μ L and 750 μ L of solution into a 5 mm NMR tube.
- 2 Gently insert the NMR tube into a sample turbine. This is most easily accomplished by placing the empty turbine into the top of the sample depth gauge and then gently sliding the tube into the hole in the top of the turbine. Gently push the tube down until the sample just touches the bottom of the depth gauge. This step insures that the sample will be positioned in the probe coil after insertion into the magnet. **Remove the sample/spinner combination from the depth gauge.**
- 3 The next step is to load your sample into the robot tray. **Care must be taken to avoid blocking the location reserved for the sample currently in use.**
7600-AS: The current location will be displayed on the LCD information panel.
7510-AS: The location directly over the magnet bore is reserved for the sample currently in the magnet and should not be used.
4. Insert the sample into the next open location and note the location.
- 5 If the VnmrJ window is not already showing the **Standard** panel, click on the **Start (5)** tab and then click the **Standard** panel (immediately below the Start tab) to navigate the point of view to that page.
- 6 If the sample tray display is not visible, use the Automation -> Tray Actions -> Show Tray menu option to open it. (The 7510-AS tray display will only have 12 positions.)
- 7 Next, click on the **New Study (7)** button. This will reinitialize the sample display and move the software into Study Mode. While in this mode, the software allows the user to build a queue of experiments for a sample, then customize the parameters associated with those experiments and the actions to be performed on the sample.



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- 8 Click the location in the tray display that corresponds to your sample. (For the 7600-AS, the row and column designations are shown on the side and bottom of the display, respectively.) The selected sample location will now show a flashing highlight ring.
 - 9 Next, fill in the information associated with your sample, such as **sample name**, **solvent**, sample numbers, comments about the sample, etc. The sample name parameter is typically required as part of the automatic data saving routine and the solvent information is used to set the spectral window appropriately.
 - 10 Click on the button(s) in the Experiment Selector, such as **PROTON**, that correspond to the experiments you wish to collect on your sample. Navigation between the available experiment buttons is accomplished by clicking on the various tabs in the Experiment Selector window. (The wet1D and PRESAT experiments require sample-specific customization and should not be used before consulting Chapter 5, "Using Studies," in the Automation Manual.)
 - 11 Each experiment will be added to the Study Queue as individual nodes.
 - 12 Once the Study Queue has been built with the desired experiments, click **Submit**. The same Study Queue can be submitted to multiple samples by changing the sample information, selecting the location of the next sample, and clicking the Submit button again.
 - 13 Click **Done** to exit Submit Mode.
 - 14 Progress can be monitored in the Acquisition Status window. The display will show a series of tasks being performed, interspersed with periods of "Idle" while the system is waiting for a process to complete.
 - 15 Progress can also be monitored in the Study Queue window. Selecting the **Spectrometer** view by choosing "Spectrometer" from the drop-down list will display nodes for all samples in the current automation run, while selecting the "Active Sample" view will just display the list for the sample currently running in the magnet.
 - 16 Note that completed nodes are green, the active node is blue, and queued nodes are yellow. Other colors, denoting other sample conditions, are also possible.
 - 17 Dragging a completed **Experiment Node** to the graphics window will automatically process that data set and load it into the current experiment space.



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- 18 Click on the **Process** tab to display the various data manipulation panels.
 - 19 Click on the **Plot** panel to display the plotting tools. Simple plotting tools are also available on the **Basic** panel.
 - 20 Use the graphics toolbar to adjust the displayed spectrum as desired. Hovering the mouse over the icons will display tool tips. In particular, select the “magnifying glass” then click and drag the cursor across the spectrum to zoom in on a region of interest.
 - 21 Click **Auto Plot Preview** to render a plot of the spectrum. The plot will be a duplicate of the spectrum as displayed in the graphics window. The data will be opened in a new Adobe® Reader® window.
 - 22 Review the formatted plot in the Adobe Reader window. Repeat steps 20 -21 as needed to adjust the results.
 - 23 Once the plot is displayed as desired, use the check boxes in the PlotView popup window to send the plot to a printer, a pdf file, or as an e-mail attachment if the Linux® e-mail tools have been configured.

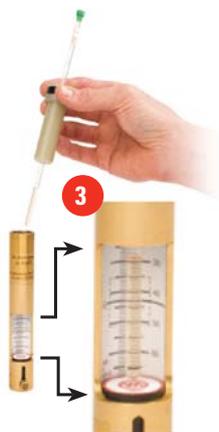


Collecting data on systems without a Robot Sample Changer

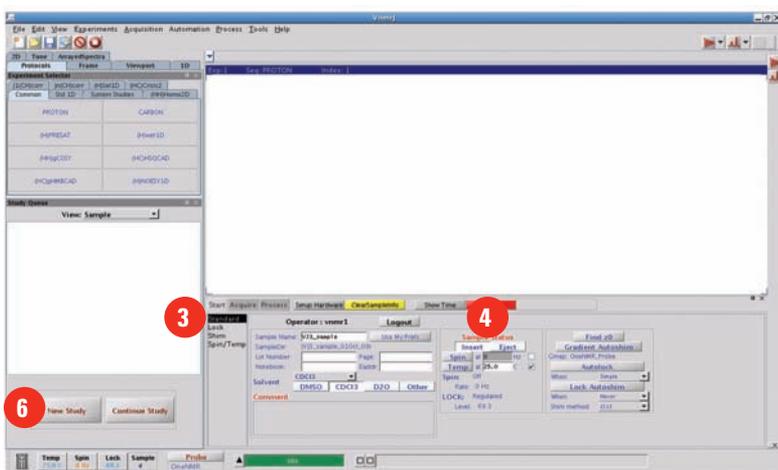
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2. Gently insert the NMR tube into a sample turbine. This is most easily accomplished by placing the empty turbine into the top of the sample depth gauge and then gently sliding the tube into the hole in the top of the turbine. Gently push the tube down until the sample just touches the bottom of the depth gauge. This step insures that the sample will be positioned in the probe coil after insertion into the magnet.

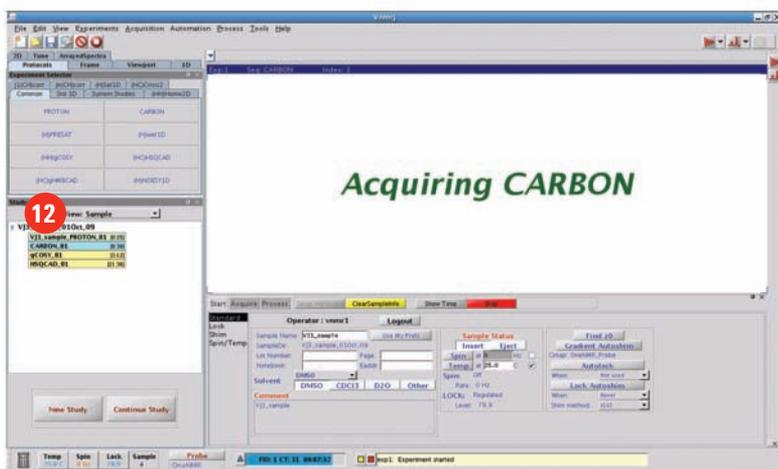
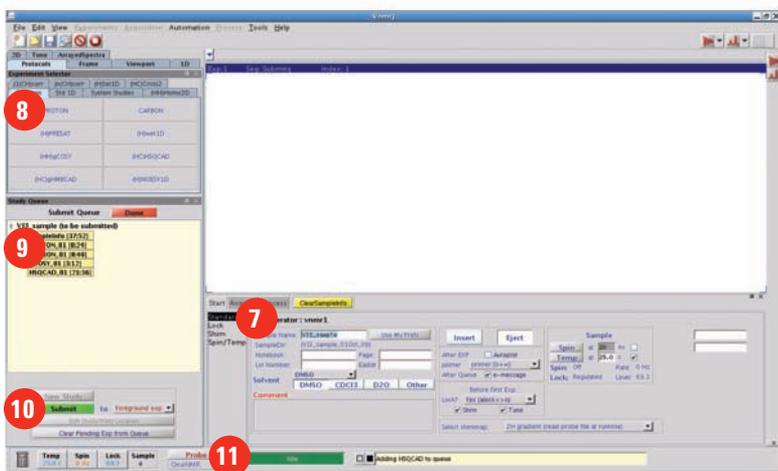
Remove the sample/spinner combination from the depth gauge.



3. If the VnmrJ window is not already showing the **Standard** panel as depicted above, click on the **Start** tab and then click the **Standard** panel (immediately below the Start tab) to navigate the point of view to that page.
4. Click on the **Eject** button to lift the current sample from the magnet.
5. The current sample will lift out of the magnet. Carefully remove the current sample and replace it with the new sample. The sample will float on top of the upper barrel until the **Insert** button is clicked. The new sample will now gently lower into the magnet.
6. Next, click on the **New Study** button. This will reinitialize the sample display and move the software into Study mode. While in this mode the software allows the user to build a queue of experiments for a sample, then customize the parameters associated with those experiments and the actions to be performed on the sample.



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- 7 First, fill in the information associated with your sample, such as **samplename**, **solvent**, sample numbers, any comments about the sample, etc. The samplename parameter is typically required as part of the automatic data saving routine, and the solvent information is used to set the spectral window.
 - 8 Click on the button(s) in the Experiment Selector, such as **PROTON**, that correspond to the experiments you wish to collect on your sample. Navigation between the available experiment buttons is accomplished by clicking on the various tabs in the Experiment Selector window. (The wet1D and PRESAT experiments require sample-specific customization and should not be used before consulting Chapter 5, "Using Studies," in the Automation Manual.)
 - 9 Each experiment will be added to the Study Queue as individual nodes.
 - 10 Once the Study Queue has been built with the desired experiments, click **Submit**. The spectrometer will begin by adjusting the Z0 offset, shimming the sample, and setting the receiver gain automatically before collecting the requested data.
 - 11 Progress can be monitored in the Acquisition Status window. The display will show a series of tasks being performed, interspersed with periods of "Idle" while the system is waiting for a process to complete.
 - 12 Progress can also be monitored in the Study Queue window. Selecting the "Active Sample" view from the pull-down menu will display the experiment list for the current sample. Note that completed nodes are green, the active node is blue, and queued nodes are yellow. Dragging a completed **Experiment Node** to the graphics window will automatically process that data set, load it into the current experiment space, and display the processed spectrum in the graphics window.



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- 13 Click on the **Process** tab to display the various data manipulation panels.
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 - 17 Review the formatted plot in the Adobe Reader window. Repeat steps 15 and 16 as needed to adjust the results. The plot might open behind the VnmrJ window. If so, just click on the Adobe Reader button in the taskbar at the very bottom of the screen to bring it to the top.
 - 18 Once the plot is displayed as desired, use the check boxes in the PlotView popup window to send the plot to a printer, a pdf file, or as an e-mail attachment, if the Linux® e-mail tools have been configured.

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Published in USA, March 18, 2011

5990-7606EN

