Agilent VnmrJ 3.2

Quick Start Guide

This Quick Start Guide describes how to acquire NMR spectra using Agilent VnmrJ 3.2 software.

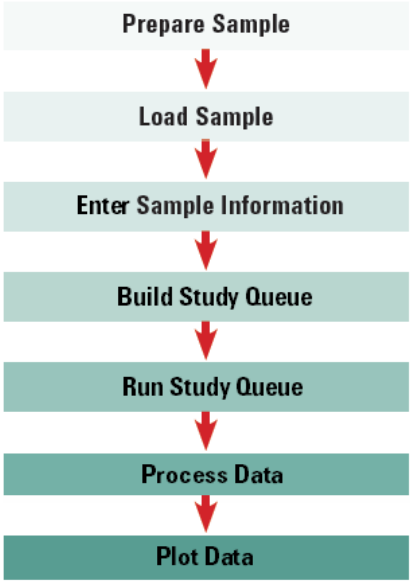
Agilent Technologies

VnmrJ 3.2 Interface

Overview

Collecting an NMR spectrum requires just a few quick steps:

- Prepare Sample–dissolve the sample then transfer the sample to an NMR tube. Position the NMR tube at the appropriate depth in the spinner turbine.
- Load Sample–place the sample into the magnet or into a location in the robot tray.
- Enter Sample Information–fill in sample information, including sample name and solvent.
- Build Study Queue–select experiments to be run on the sample.
- Run Study Queue–run selected experiments on the sample, or on multiple samples with a robot sample changer.
- Process Data–use the data processing tools to optimize the spectrum display.
- Plot Data–use the plotting tools and Graphics Toolbar to adjust the displayed spectrum for the desired output.



Prepare Sample

1. Prepare the NMR sample by dissovling the analyte in a deuterated solvent.

   Use a concentration that will completely dissolve the sample, usually between ~1 mg/mL and ~50 mg/mL.

2. Transfer between 600 µL and 750 µL of the solution into a 5-mm NMR tube.

3. Positioning the NMR tube:

   a Insert the NMR tube into a spinner turbine.

   b Carefully place the spinner turbine into the top of the sample depth gauge

   c Carefully push the NMR tube through the turbine until the NMR tube slightly touches the bottom of the depth gauge.

Depth gauge

   d Remove the spinner-turbine from the depth gauge.

   This step insures that the sample is positioned in the probe coil after insertion into the magnet.

Load Sample

4 Load the sample into the system.

a Click **Eject** on the VnmrJ **Start > Standard** parameter panel to lift the current sample to the top of the magnet bore.

b Carefully remove the current sample and replace it with the new sample.

c Click **Insert** on the **Start > Standard** parameter panel to lower the sample into the magnet.

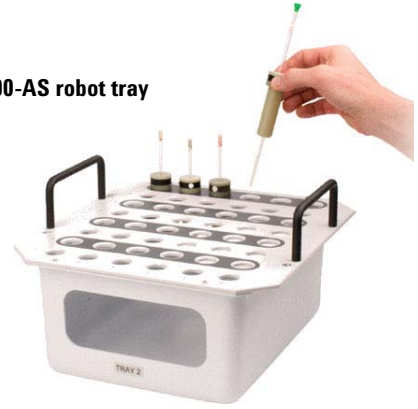
5 *For systems with a robot sample changer*:

a Load your sample into the robot tray and note the location. Avoid blocking the location of the sample currently in the magnet.

7600-AS: The current location is displayed on the LCD information panel.

7510-AS: The location directly over the magnet bore is reserved for the sample currently in the magnet.

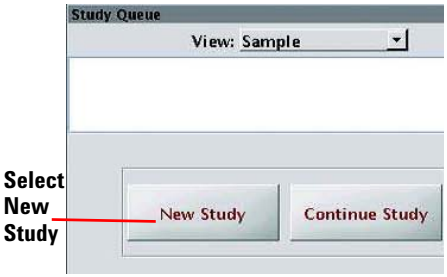
7600-AS robot tray



7510-AS robot tray

Enter Sample Information

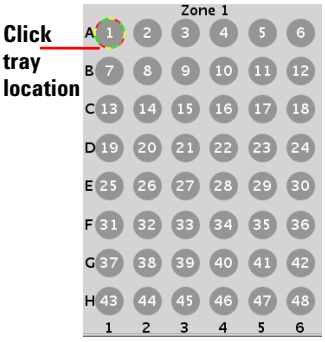
6 Select **New Study** in the Study Queue. Submit Queue will display in the Study Queue.



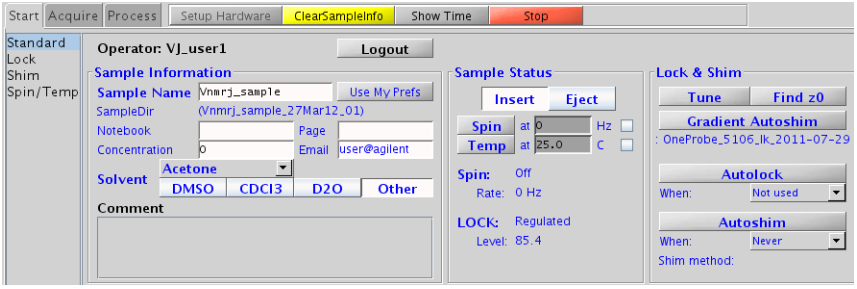
7 *For systems with a robot sample changer:* After **New Study** is selected, the sample tray display will refresh and display in the Graphics Canvas.

a Click the tray location associated with the inserted sample on the sample tray.

The selected sample location shows a flashing highlight ring. To the right, the 7600-AS, Zone 1 tray display has the A1 location selected.



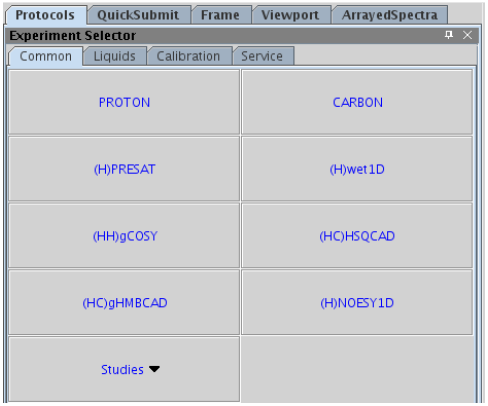
8 Fill in sample information on the **Start > Standard** parameter panel.



Sample Name and Solvent are required fields. Sample Name is used in the automatic data saving routine. Solvent is used to set the spectral window. Filling out additional sample information is good practice.

Build Study Queue

9 Select the **Protocols** vertical panel to access the **Experiment Selector**.



10 Select Experiments from the Experiment Selector tabs to run on the selected sample.

Each experiment will be added to the Study Queue displayed as a node.

Run Study Queue

11 Click Submit to run the Study Queue.

The Acquisition Status display on the hardware toolbar shows: the task being performed, time left for the task to run, **Idle** when waiting for a process to complete, or **Inactive** when no process is being run.

The Study Queue experiment nodes appear green if completed, blue if active, and yellow if queued.

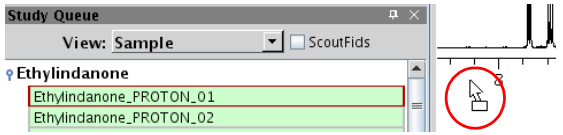
NOTE

For systems with a robot sample changer:
The same Study Queue can be submitted to multiple samples by: changing the sample information, selecting a sample-tray location, and clicking **Submit**.

Process Data

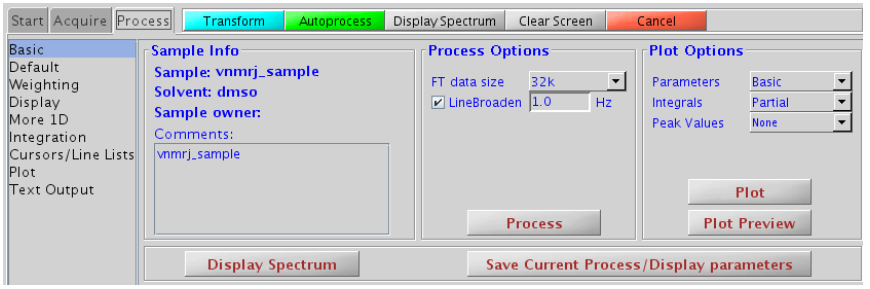
12 Select and drag a completed experiment node to the Graphics Canvas to automatically process and load the data set.

In the example to the right, "Ethylindanone_Proton_01" has been selected from the Study Queue and is being dragged to the Graphics Canvas.



13 Click on the **Process** tab to display the data manipulation tools.

Basic processing tools are available on the **Process > Basic** parameter panel.



Plot Data

14 Click **Process > Plot** to display the plotting tools.
Basic plotting tools are available on the **Process > Basic** parameter panel.

15 Use the Graphics Toolbar to adjust the displayed spectrum.
Hovering the mouse over the icons displays tool tips.

16 Click **Plot Preview** to render a duplicate of the displayed spectrum in Adobe Reader.
The **Plot View** dialog box appears.

a Review the formatted plot and readjust as needed.

17 Select one or more check boxes on the **Plot View** dialog box to print, save as a PDF file, or email the plot.

www.agilent.com

In this book

This Quick Start Guide provides a step-by-step overview of how to use Agilent VnmrJ 3.2 software to collect an NMR spectrum on NMR systems with or without a Robot Sample Changer.

April 2012

G5028-90018

Agilent Technologies