

VNMRJ 4.2

Quick Setup

After Clicking VNMRJ Icon

2. Click Yellow Cross

The screenshot shows the VnmrJ software interface with several panels and a central graphics canvas. A blue arrow points to a yellow 'X' icon in the top right corner of the window. Another blue arrow points to a checkbox labeled 'Show this Help Overlay on Startup' in the bottom left corner.

Experiment Selector
Choose one or more experiments to run now in the foreground, or configure experiments to run later in the Study Queue.

Use the other Vertical Panels to display and manipulate multiple spectra side by side or in overlay.

Command Line Use the command line for direct access to VnmrJ commands, macros and parameters.

Graphics Canvas
Spectra are displayed in this area. Interact with your data using the tools in the Graphics Toolbar to perform zooming and panning, adjust vertical scale, find and display integrals and pick peaks.

Experiment Parameter Panels
Use the Experiment Parameter Panels to configure acquisition parameters and to control details of the measurement workflow such as when to perform autoshimming. Parameters from one experiment can be carried over to related experiments for easy setup. The panels also include facilities to control the hardware, including setting spin rate and temperature. The Parameter Panels are organized into tabs, and each tab contains one or more pages. For example the Process Tab provides options for spectral processing and plotting. The Action Bar provides quick access to commonly used functions for the task at hand.

Hardware Toolbar
Shows the status and history of temperature, spin rate and lock strength, and displays the location of the active sample.

Acquisition Status
Indicates the current acquisition task being performed and displays the time remaining for the acquisition to complete.

Message Box
Toggle between the display of software and hardware messages.

Graphics Toolbar
1D Zoom
1D Integral
1D Phasing
Redraw
Return

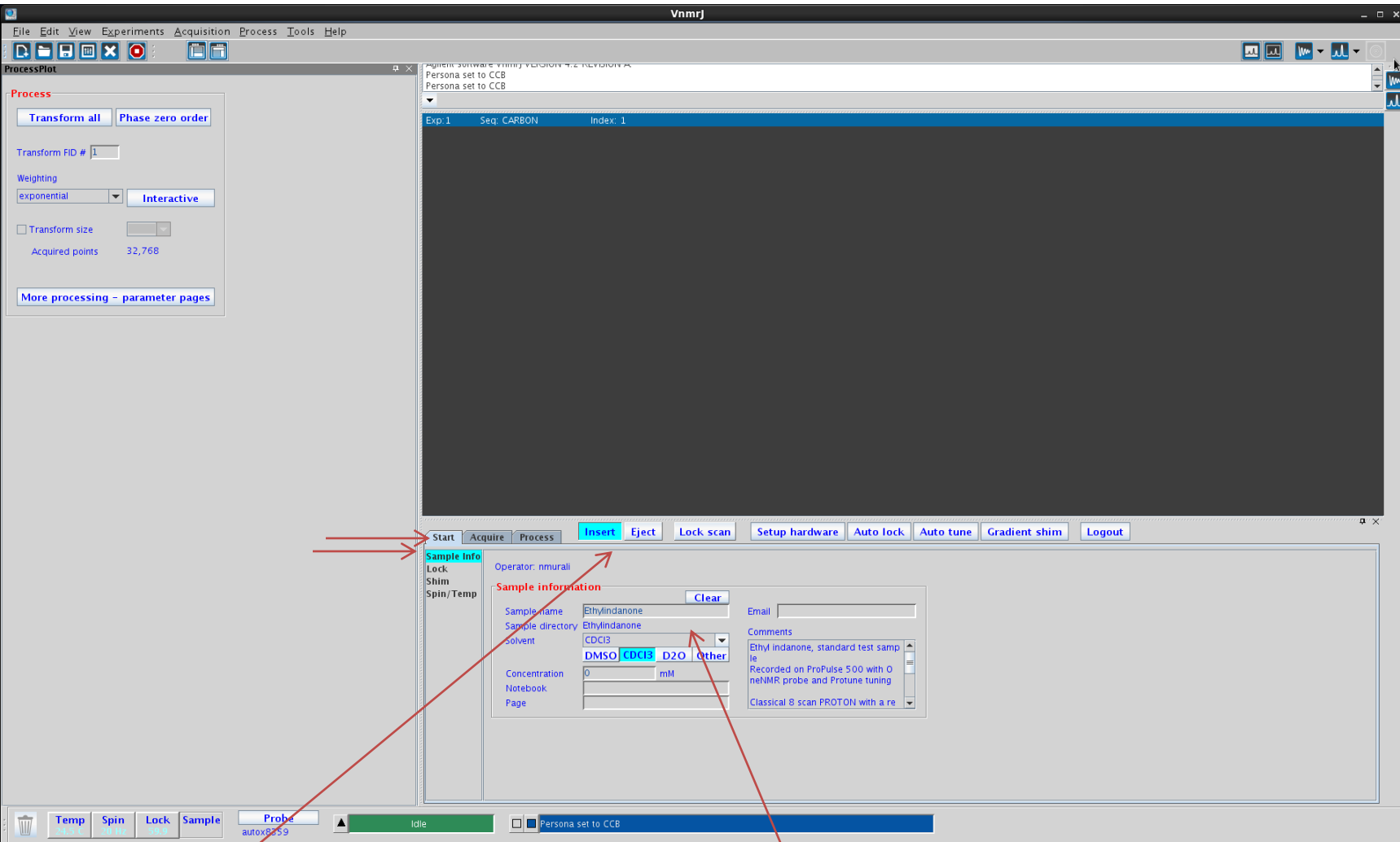
Annotations:
- A yellow box highlights the 'Action Bar' and 'Parameter Panels' in the Experiment Parameter Panels section.
- A yellow box highlights the 'Pages' and 'Parameter Panels' in the Experiment Parameter Panels section.
- A yellow box highlights the 'Tabs' and 'Action Bar' in the Experiment Parameter Panels section.

Peak Data from Graphics Canvas:

Chemical Shift (ppm)
8.38
7.97
5.43
4.87
4.59
3.85
3.75
3.18
2.95
2.86
2.36
1.52
0.92
0.00

1. Uncheck this box

Sample Insert/Eject & Solvent

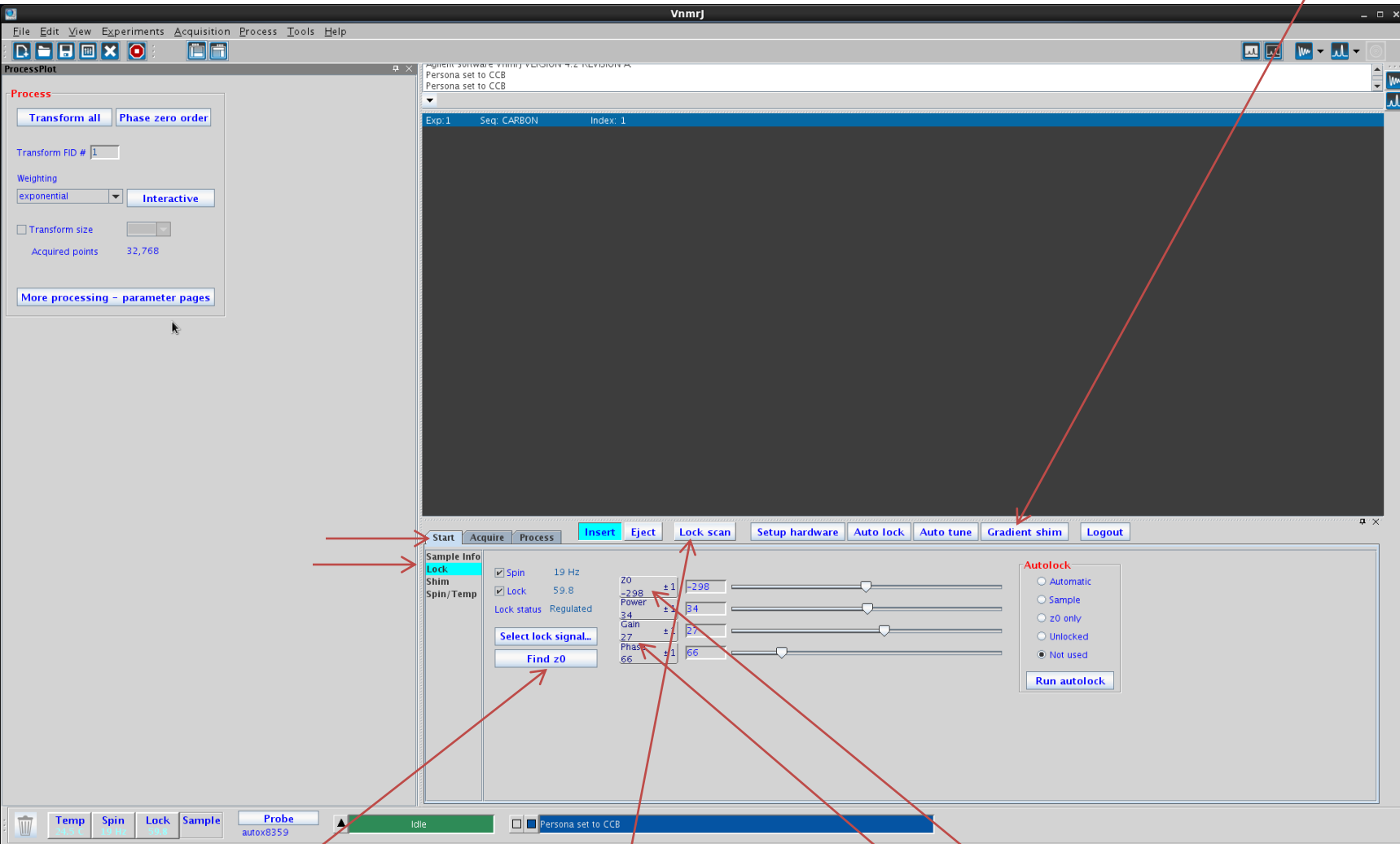


1. Insert/Eject buttons

2. Set Solvent name here

Lock & Gradient shim

3. Click **Gradient Shim** for shimming

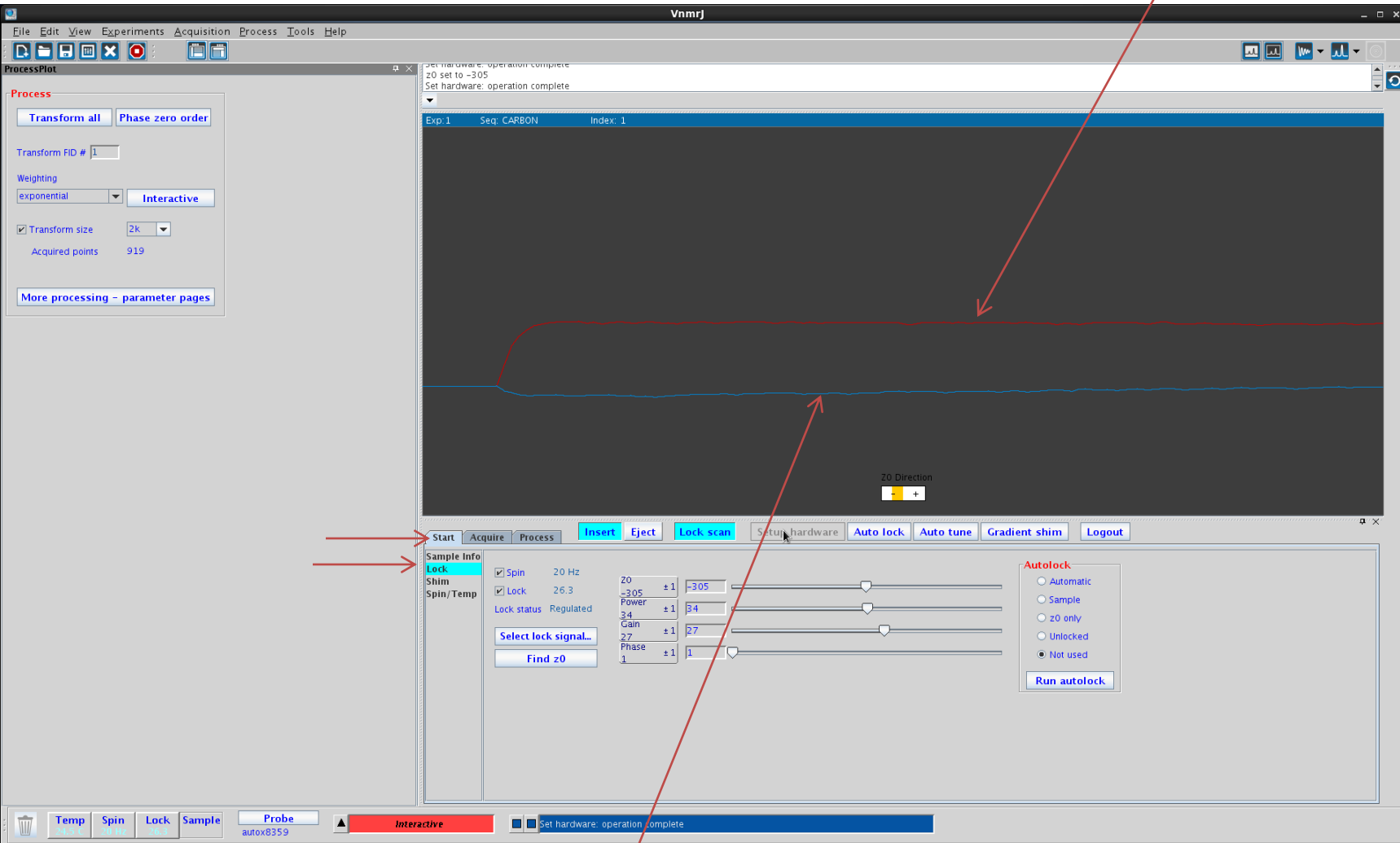


1. Click **Find Z0**

2. Click **Lock Scan** to adjust Phase & Z0 – Not needed in this software.

Lock Display

Lock Line (Red)



Phase Line - Blue

Select the experiment from
Experiments Menu

Select Experiment

The screenshot displays the Vnmrj software interface. The top menu bar includes 'File', 'Edit', 'View', 'Experiments', 'Acquisition', 'Process', 'Tools', and 'Help'. The 'ProcessPlot' window is active, showing a list of experiments with 'Exp. 1' selected. The 'Process' tab is selected, displaying acquisition parameters such as 'Spectral width (select)', 'Number of scans', 'Relaxation delay', and 'Pulse angle'. The 'Experiments' menu is highlighted, and a red arrow points from it to the 'Exp. 1' entry in the plot area. Another red arrow points from the 'Process' tab to the 'Acquisition options' section.

Experiment Name

Auto Tune

The screenshot displays the Vnmrj software interface. The main window shows a 'ProcessPlot' area with a dark background. Below this, there is a menu bar with buttons: Start, Acquire, Process, Insert, Eject, Lock scan, Setup hardware, Auto lock, Auto tune, Gradient shim, and Logout. The 'Auto tune' button is highlighted in blue. Below the menu bar is a 'Sample Info' section with fields for Sample name (Ethylindanone), Sample directory (Ethylindanone), Solvent (CDCl3), Concentration (0 mL), and Notebook/ Page. The 'Auto tune' button is also highlighted in the 'Process' menu. Two red arrows point from the 'Start' folder and the 'Auto Tune' button to the text below.

Click on **Start** folder and then click on **Auto Tune** button. This is done after selecting experiment.

Acquire Data

The screenshot shows the Vnmrj software interface. The main window displays the acquisition setup for an experiment named 'PROTON'. The 'Acquire' folder is highlighted in the left sidebar, and the 'Go' button is highlighted in the top toolbar. The 'Acquisition options' section is visible, showing parameters such as 'Spectral width (select)', 'Number of scans', 'Relaxation delay', and 'Pulse angle'. The 'Go' button is highlighted in red, and a red arrow points from it to the instruction text below. Another red arrow points from the 'Acquire' folder in the sidebar to the same instruction text.

Agilent software Vnmrj VERSION 4.2 REVISION A
Persona set to CCB
Persona set to CCB

Exp: 1 Seq: PROTON Index: 1

Start Acquire Process Show time Go Stop MoveSW Est. pw90 Arrays Sequence diagram Sequence help

Default m1
Acquisition
Pulse Sequence
Channels
Flags
Future Actions
Overview

Experiment: PROTON Solvent: d2o Observe: H1 Decoupler: C13
Receiver gain (dB) 20
 Autogain

Acquisition options
Spectral width (select) -2.0 to 14.0 ppm
(..or enter) ppm
Number of scans 1
Relaxation delay 1 s
Pulse angle 45 degrees

Temp Spin Lock Sample Probe
Idle Persona set to CCB

Click on **Acquire** folder and then set desired number of scans etc... Then click **Go** button.

Process Data

1. After acquisition from GO spectrum is displayed. Click on **Process** folder.

Click on **Plot** and then select options. Check **Print Double-Sided**. Then **Click Print**.

Save Data

The screenshot displays the Vnmrj software interface. The main window is titled 'Process-Plot' and shows a spectrum plot with a prominent peak at approximately 4.7 ppm. The x-axis is labeled 'ppm' and ranges from 0 to 9. The y-axis is labeled 'V_position' and ranges from 0 to 552.5. The plot is titled 'Exp: 1 Seq: PROTON Index: 1'. The interface includes several panels and buttons:

- Process:** Buttons for 'Transform all' and 'Phase zero order'. A 'Transform PD #' field is set to 1. Weighting is set to 'none' and 'Interactive' is selected. 'Transform size' is 2k and 'Acquired points' is 16,384. A 'More processing - parameter pages' button is present.
- Display:** 'Vertical scale' is set to 'Autoscale' and 'Arrayed spectra panel' is selected. Reference is set to 'By solvent' and 'By TMS'. 'Display mode' is set to 'phased'. A 'More display - parameter pages' button is present.
- Plot:** Buttons for 'Auto plot', 'Auto preview', and 'Print screen'. A 'More plotting - parameter pages' button is present.
- Process Panel:** Includes 'Spectral graphics' (Current checked, Full array unchecked, FID unchecked), 'Logo' (Agilent, Custom, None), 'Integral lines' (Full, Partial, None), 'Integral values' (Scaled, Normalized), 'Peak labels' (ppm, Hz), and 'Peak positions' (ppm, Hz). 'Comments' and 'Miniplots' are checked.
- Send to:** A dropdown menu and 'Print double-sided' checkbox. 'Preview' and 'Print' buttons are available.
- Status Bar:** Shows 'Temp', 'Spin', 'Lock', 'Sample', 'Probe' (autox8359), and 'Idle'.

Save data from the **File** menu.

Exit/ Logout

- Exit VNMRJ from **File** menu.
- From **System** menu on the **Desktop** select logout.