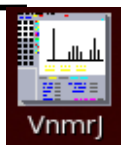
v1.3

Duke UNIVERSITY NMR Center

Quick start guide for routine **1D PROTON/CARBON** experiment

Instrument: 400 VNMRS



1) **Log In:** Log into your user account.

2) **Launch VnmrJ:** Launch **VnmrJ** software using the icon on the desktop.

3)

4) **Insert sample:** Turn off lock, type **e** to remove the standard sample. Place your sample in the spinner, wipe with Kimwipe, place your sample in the spinner and back into the magnet on the bed or air. Type **i** to insert. Make sure **spin** is on (20 Hz).

5) **Lock:** Under the Start tab and Sample Info, **select your solvent**. Enter sample information into the comment section.

6) **Adjust Z0:** Turn **lock scan** on, adjust **Z0** to maximize square wave.

7) **Shim:** Turn on **lock**. Then, navigate to the Start / Shim tab. Maximize the value of the lock level, indicated by the dial, by changing the **Z1C, Z2C, Z1 and Z2** shims only! (DO NOT TOUCH ANY OTHER SHIMS).

8) **Load in proton experiment and parameters:**
   i) Select **Experiments -> Proton** (or **Carbon**)) to load the default proton. **--or--**
   ii) Open a saved 1D ^{1}H experiment (or 1D ^{13}C). Click the **Open** icon. Type: **load='y' su**

9) **Check important acquisition parameters:** Block size (bs), pulse width (pw), number of scans (nt), spectral width (sw), recycle delay (d1), etc.

10) **Start the experiment:** Type **ga** or **go**, or select the **Acquire** button.

11) **Processing:** Perform a weighted FT by typing **wft f full aph vsadj vp=15 lb=1**

If no manual phasing, peak picking, integration, or plotting needs to take place please skip to step 15.

12) **Manual phase adjustment:** Select the **Adjust Phase** button. Left-click and hold on the most upfield peak. Move the cursor up or down. Then repeat with the downfield region.

13) **Peak picking:** Define the peak threshold using the **Show/Hide Threshold** button, and using the left mouse button to define the threshold. Peaks that show above the defined threshold will be found for peak picking. Hit the **Pick Peaks** button.

14) **Integration:** Navigate to the Process / Integration tab. Enter Integration mode using the **Integration** button. Defining Integration Regions: To define your true integration regions, use the left mouse button (LMB) while in **Cut Integrals** mode, and click once on the left side of your peak, and again on the right side of your peak (repeat as needed). Calibrating Integrals: LMB to select the integral you will use for calibration. You should have only one red cursor through the selected integral. Then under the Set Integral Area option, select **Single Peak**, and set the desired integral value.

15) **Plotting:** To create a hard plot, type: **pl pscale pir ppa page**

16) **Saving:** To save your FID, hit the **Save** icon.

17) **Remove your sample:**

18) **Logout:** Close VnmrJ (**File -> Exit VnmrJ**). Log out of your Linux user account. Clean up the workspace.

Green = clickable command

Red= typable command

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