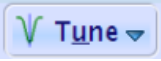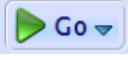# Acquiring ^{19}F 1D Experiments on the Bruker NMR

by Monika Ivancic, PhD (October, 2020)

1. Start by acquiring a ^{1}H 1D experiment (uvm.1H1D) (see Bruker Speedy setup guide) Even if you may not need the data, a ^{1}H 1D will be the best indicator of shim quality. Also, for X-nuclei spectra, one can reference these spectra from a ^{1}H spectrum that was acquired under identical lock conditions (so same lock and shim), which can only be true in the same session. You may use NS = 8, which will take less time.

2. Create a new dataset (type 'new' to get GUI up), set experiment number to 2, then for experiment, choose 'uvm.19F' (no ^{1}H decoupling) OR 'uvm.19F.dec1H' (with ^{1}H decoupling), depending on whether or not you want the ^{1}Hs decoupled. You may acquire both versions and compare the differences.

3. Tune the probe to ^{19}F by typing 'atma' or clicking **√ Tune ▼**. The system will tune ^{19}F at about 470.5MHz. It may or may not retune ^{1}H after. Please be patient, it's important for the process to finish.

4. Optimize receiver gain by typing 'rga' or clicking on **⌐ Gain ▼**. ^{19}F is almost as sensitive as ^{1}H, and is a great nucleus to study by NMR.

5. Acquire your data by typing 'zg' or clicking **▶ Go ▼**. This is a short, 8 scan experiment. Once acquisition is complete, type 'efp'. You should get a warning GUI about this being a digitally filtered dataset. Please ignore warning. Then type 'apk', although spectrum may remain out of phase. Don't worry about it, since we're re-acquiring below.

   The default experiment uses a large sweep width (SW = 241.5ppm) and is centered at O1 = -100ppm. It is important to reduce this SW, in case your peak has finer coupling that wouldn't be picked up with this large SW.
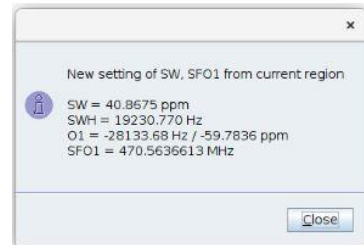
6. You are going to keep the data that you acquired in 5. Copy the dataset (includes parameters AND data) into another experiment by typing 'wra 3' (copy into experiment 3) and then you need to go into that experiment by typing 're 3'. At this point it will look identical, but above your data and tabs, you will see what experiment number you're in.

   Here is an example of being in exp 1:

7. Adjust the sweep width to be about 20-40ppm surrounding your peak. If you have more than one peak, make sure the new sweep width includes all the peaks with enough baseline (~5ppm or more) to the left of the leftmost and to the right of the rightmost peaks. Using the mouse, left-click at the starting point (and hold) until the end point. The zoomed in spectrum will appear when you release.

8. Then click the icon, which adjusts the SW and O1 parameters. You will get a message like this:

New setting of SW, SFO1 from current region

SW = 40.8675 ppm
SWH = 19230.770 Hz
O1 = -28133.68 Hz / -59.7836 ppm
SFO1 = 470.5636613 MHz

Close

9. Re-acquire the data with 'zg' or , this data will have the new SW and O1. Then process with 'efp' (you may get the same warning as in 5, just ignore) and use 'apk' to phase data, which should phase properly this time.

10. If you followed the above instructions, you will have 3 datasets:

Exp 1 – a ^{1}H 1D

Exp 2 – a ^{19}F with a large SW

Exp 3 – a ^{19}F with the smaller adjusted SW

11. If you acquired a 'uvm.19F' in the above instructions, you may repeat with a 'uvm.19F.dec1H'. By comparing the two, you will be able to determine whether or not ^{1}Hs are splitting the ^{19}F peak.