Referencing NMR Spectra

This page discusses how to reference NMR spectra of any type acquired on the Agilent 600 MHz instrument.

Referencing ^{1}H Spectra or ^{1}H Dimensions in Multi-dimensional Spectra

1. First, acquire a 1D ^{1}H NMR spectrum at the temperature and conditions in which you recorded the spectrum of interest. Before you start set **tof=0**. Find the top of the peak of the water resonance using the cursor. Then type **movetof**. Note the new value of tof.
2. Record 1D ^{1}H NMR spectrum for your sample using the new value of tof. Determine the chemical shift of the water resonance in ppm using the formula: **delta = 7.83 - [temp (in Kelvin)/96.9]**. If you are referencing your ^{1}H spectrum in Felix, note where the water resonance is (in points) and then enter this value and that of the water chemical shift for the reference point and the reference shift parameters, respectively, in the reference matrix window.

Referencing Indirectly Recorded ^{15}N or ^{13}C Dimensions

1. First, acquire a 1D ^{1}H NMR spectrum at the temperature and conditions in which you recorded the spectrum of interest. Before you start, set tof=0. Find the top of the peak of the water resonance. Then type **movetof**. Note the new value of tof.
2. Now check the value of sfrq by typing **sfrq?** in Vnmrj or by searching for it in the procpar file if you have already recorded the 1/2/3D data. This is the carrier frequency and it corresponds typically to the frequency of the water resonance in Hz. Determine the chemical shift of the water resonance in ppm using the formula: **delta = 7.83 - [temp (in Kelvin)/96.9]**. Now multiply the carrier frequency with **(1 - [delta/1000000])**. This is the absolute frequency of a hypothetical resonance at 0 ppm.
3. Now multiply this frequency with **0.251449530** (for ^{13}C) and **0.101329118** (for ^{15}N). These are the corresponding absolute frequencies of the corresponding 0 ppm values for the ^{13}C and ^{15}N dimensions, referenced relative to DSS. See this page for more information regarding IUPAC-IUB recommended chemical shift ratios.
4. Most likely, you have already run your experiment with **dof** or **dof2** set to appropriate values. Now you need to find what the chemical shifts these correspond to. Fortunately, in the new version of Vnmrj the carrier frequency (in Hz) is reported under **dfrq** or **dfrq2**, which you can either get by typing **dfrq?** or **dfrq2?**. Alternatively, get the values for **sfrq/dfrq/dfrq2** from the procpar file by searching for these strings. Then divide the carrier frequency with the absolute frequency in MHz at 0 ppm. Subtract **1.0000000** from the result and multiply with **1000000**, and viola, you have the chemical shift in ppm at the carrier frequency.