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Performing the 1D ^{1}H-^{19}F NOE Experiment

This document describes how to set up a 1D, selective, steady-state NOE between ^{1}H and ^{19}F using the normal s2pul pulse sequence.

A: Data Collection

(1) In exp1, setup a normal **^{1}H** experiment, collect a ^{1}H spectrum; probably save it
(2) In exp2, setup a normal **^{19}F** experiment, collect a ^{19}F spectrum; probably save it
(3) Type **dn='F19'** on the command line
(4) Put the cursor in the center of the ^{19}F peak of interest and type **nl**
(5) Type **sd** to give a dof value for ^{19}F. **Write down the dof value.**
(6) If you have more than one Fluorine peak that could potentially give the NOE to protons, repeat step 4 and 5 for all the peaks. **Write down all the dof values.**
(7) Move the parameters in exp1 to exp3 by the commands: **mf(1,3) jexp3 wft**
(8) In exp3, make sure
dn='F19'
d1=2 (can be set longer e.g. 5s)
d2=5 (can be set longer e.g. 10s)
homo='y'
gain='y'
dm='nyn','nnn'
dmm='ccc', dmf=200 dpwr=10
dof=the value found in exp2 (step 5 or 6 above)
Collect ^{1}H spectrum with the desired nt (number of transients)

(9) Type **da** to look at the arrayed values and **dg** to go back to the normal parameter display
(10) You can array **dpwr** value to find the best saturation power for obtaining NOE peaks (in this case, don't array dof, use just one dof value found above to avoid complications). Normally, dpwr=10 should be good enough and don't use a number larger than 10. Once you have a desired **dpwr** value, collect the selective NOE between ^{1}H and ^{19}F spectrum as in step (8).
(11) Once you are done with the data collection, save the data which contains 2 spectra
(12) If you have multiple ^{19}F peaks and dof values, repeat step (7) to (11) in a different experiment window for instance, type **mf(1,4) jexp4 wft** (Don't use exp5).

B: Data Processing

(1) Process the arrayed data as usual (**proc** or **wft aph** or use manual phasing)
(2) Type in the command line: **clradd ds(1) add ds(2) sub jexp5** (these macros delete experiment window 5 (exp5), and then create exp5, add spectrum #1 to exp5, then subtract the spectrum #2 from #1)
(3) Go to exp5: jexp5 wft to see the resulting spectrum, only the ^{1}H peaks which have NOE with the ^{19}F signal show up, the other ^{1}H peaks are subtracted to zero (note: there may be small residual peaks if the lower number of scans are used (more than 32 scans is recommended).
(4) You can save this resulting NOE spectrum as usual.
(5) Note: above commands (**clradd ds(1) add ds(2) sub jexp5**) can be replaced by a macro by typing: **hfnoe** (vxr500 only)
(6) Or you can process the NOE spectrum in Mnova using Arithmetic tool under Analysis menu