

## Heteronuclear Decoupling

Decoupling attached heteronuclear spins is a common event in many NMR experiments and there are several parameters that control correct decoupling setting and it is useful to know them and their function.

For every channel there are a set of parameters that have same syntax with the channel number added:

Channel 2/1 <sup>st</sup> Decoupler	Channel 3/2 <sup>nd</sup> Decoupler	Channel 4/3 <sup>rd</sup> Decoupler
dpwr	dpwr2	dpwr3
dm	dm2	dm3
dmm	dmm2	dmm3
dmf	dmf2	dmf3
dres	dres2	dres3
dseq	dseq2	dseq3

The description for Channel 2 is sufficient as it is same for other channels also.

### INOVA spectrometer

Assuming one knows the pw90 value on the decoupling channel at the power level, the following are the steps to set correct decoupling values manually. If you do not know the power/pw calibration, use attval macro to find it.

- (1) Set dpwr to the power level
- (2)  $dmf = 1.0/pw90$  and this essentially sets  $dmf = 4 * \gamma_{B_2}$  for that channel. Beware pw90 is in  $\mu s$  units, use the value explicitly (for e.g. 40e-6)
- (3) dm is the decoupler status 'y' means on. If status C is acquisition time then  $dm='nny'$
- (4) dmm is the modulation mode:  $dmm='ccw'$  means the modulation mode is cw in status A & B but waltz-16 in C. The commonly used values are c, w, m, g, x for cw, waltz-16, mlev-16, garp, and xy32. In this mode, it is not necessary to set dres or dseq
- (5) dmm can also take value p such as  $dmm='ccp'$  so that decoupling is done by a waveform using waveform generator in the console. Then one should set dres and dseq also.
- (6) dres is the fine tip-angle resolution and depends on the waveform used. The value of dres range from 1 to 90 depending on the waveform used to decouple.
- (7) The name of the decoupling waveform is set by the parameter dseq. For  $dseq = 'waltz16'$  set  $dres=90$ . There should be a file waltz16.DEC either in local `vnmsys/shapelib` directory or in `/vnmr/shapelib` directory. The standard files in `/vnmr/shapelib` are waltz16.DEC, mlev16.DEC, garp1.DEC, xy32.DEC. The dres values are 90,90,1,90 respectively. Note when dseq is set the .DEC extension is not used.
- (8) When programmable decoupling is used, the shapes are created using Pbox. In this case use the dmf, dres, and dpwr values from the shape header. The dmf may not be  $1.0/pw90$  and dres could be any value. For example wurst40N created by BioPack will have large dmf and  $dres=9.0$ .

## **VNMRS spectrometer**

With VNMRS spectrometer (800 & 900) all of the above syntaxes are valid but one should always set the correct dres value too even when step (4) of above mode is used. This is because there are no separate waveform generators in the new VNMRS console and all decoupling is initiated in the same way. When dmm='ccg' it essentially looks for the standard garp1.DEC file /vnmr/shapelib and implements it. In order for this to work correct the corresponding dres value should be set (dres=1 when dmm='ccg'). For dmm='ccw' set dres=90; dmm='ccm', dres=90. The dseq parameter is only needed when dmm has the value 'p'.

The same type of logic is used for other channels also.