Disclaimer: The programs, pulses and pulse sequences listed below have been tested and used on Bruker AVANCE III/II+ spectrometers at the Karlsruhe Institute of Technology (KIT). However, the sequences are made available without any expressed warranty. We are not liable for any potential damage that might be caused in connection with the pulse programs.

Setting up the CLIP/CLAP RESET experiment

In order to set up broadband homonuclear decoupled 1D/2D NMR spectra one has to set a few additional parameters.

1) The length of each FID chunk is given by *IN_F1* and should not be much larger than 20ms for efficient decoupling with acceptable sideband intensities. The dwell time should be chosen in a way that the spectral width in the indirect dimension (*sw1*) is a submultiple of the actual desired spectral width. Choose *TD2* in a way that the acquisition time *AQ* in the direct dimension exceeds *IN_F1* by more than a factor of 2. This will avoid that your individual FID chunks are filled with zeroes after a considerable amount of data points are cut by the macro's *convdta* command.

2) The number of data chunks is determined by *TD1*, the number of increments in the indirect dimension. The concatenated FID will therefore contain *TD1* × (*IN_F1*/*DW*) data points. The value chosen for *TD1* therefore determines the resolution of the final spectrum. Typical values are 8-32.

3) To further improve the spectral quality you are able to drop further points from the beginning of each individual FID chunk by the parameter *CNST4.* The value will be handed over to the macro in aid of reducing artefacts due to the digital filtering of the individual FID chunks. Recommended values are ≥2.

Setting up the Constant-Time CLIP/CLAP RESET

The same rules given above also apply for the Constant-Time versions. In Addition you have to set the CT period d19 to a desired value of $n/^2J_{HH}$. This value will be corrected for all pulse durations and delays according to d21, which represents the maximum time for the pure-shift evolution of the spectrum and therefore the maximum length of the final FID. TD1 × IN_F1 must therefore not exceed the duration of d21.

Using the Shaped Pulses

All pulse shapes are provided under http://www.ioc.kit.edu/luy/313.php and are described in the references given below. Note that BIRD elements containing shaped pulses also employ concurrent 90° & 180° shaped pulses that have not been J-compensated according to the BUBI procedure. The additional required 90° shaped proton pulse is included in this package (see *UR90x_600u_BW10_RF20_pm20_Hc0.999959.bruker*).

ATTENTION: All shapes are designed and robust for NMR field strengths ≤ 600 MHz. They are optimized for power levels corresponding to a 12.5 µs hard pulse on ^{1}H and a 25 µs hard pulse on ^{13}C and should be calibrated accordingly.

References

T. Reinsperger, B. Luy, „*Homonuclear BIRD-Decoupled Spectra for Measuring One-Bond Couplings with Highest Resolution: CLIP/CLAP-RESET and Constant-Time-CLIP/CLAP-RESET*", *J. Magn. Reson*. 239, 110-120 (2014), http://dx.doi.org/10.1016/j.jmr.2013.11.015

S. Ehni, B. Luy, "*A systematic approach for optimizing the robustness of pulse sequence elements with respect to couplings, offsets, and B1-field inhomogeneities (COB)*", Magn. Reson. Chem. 50, 63-72 (2012), http://dx.doi.org/10.1002/mrc.3846

S. Ehni, B. Luy, "*BEBEtr and BUBI: J-compensated concurrent shaped pulses for 1H-13C experiments*", J. Magn. Reson. 232, 7-17 (2013), http://dx.doi.org/10.1016/j.jmr.2013.04.007

For downloading the latest version of the pure-shift macro, and further information and references about pure-shift experiments based on Zangger-Sterk-type data acquisition see

http://nmr.chemistry.manchester.ac.uk/?q=node/256